MICROSCOPIC CALCULATION OF HEAVY-ION SCATTERING

by

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A thesis submitted for the degree of

Doctor of Philosophy

at the

Australian National University, Canberra

May 1980

to Cali

STATEMENT

This work is the result of a close collaboration between the author, his supervisor, Dr. B. A. Robson, and Dr. R. F. Barrett. In so far as it is possible to apportion responsibility for any particular contribution to a joint project the division was as follows: (i) the α - α problem was initiated by Dr. Robson and Dr. Barrett then all detailed analysis and calculations performed collaboratively with the author; (ii) the initial stages of the ^{16}O - ^{16}O problem were a full collaboration and after a method became clear, the calculation was completed by the author. All the GCM kernels, matrix elements and particle exchange approximations were calculated by the author and the interpretation of these results is his own. The approximate methods mentioned in the last chapter are the result of further collaboration during a recent visit by Dr. Barrett.

Some of this work is already in the literature (1) and some has been submitted to various conferences (2), (3), (4). The ^{16}O - ^{16}O work has been submitted for publication (5).

No part of this degree has been presented for a degree at any other university.

R. A. Baldock.

(R. A. Baldock)

1) R. A. Baldock, R. F. Barrett and B. A. Robson, *"Natural boundary condition methods for the microscopic treatment of composite particle scattering"*, *Nucl. Phys.* A321 (1979) 171, also *Lecture Notes in Physics* 92 ed. B. A. Robson (Springer-Verlag, Berlin, Heidelberg, New York, 1979) p. 436.

2) R. A. Baldock, R. F. Barrett and B. A. Robson, *"Antisymmetrisation effects in ^{16}O - ^{16}O Scattering"*, unpublished, presented at eighth AINSE conference, ANU, 1980.

3) R. A. Baldock, R. F. Barrett and B. A. Robson, *"Antisymmetrisation effects and inelastic channels in heavy-ion scattering"*, unpublished, presented at eighth AINSE conference, ANU, 1980.

4) R. A. Baldock, R. F. Barrett and B. A. Robson, *"Particle exchange in ^{16}O - ^{16}O elastic scattering"*, to be published in *Nucl. Phys.* A, Proceedings of the international conference on nuclear physics, Berkeley, 1980.

5) R. A. Baldock, R. F. Barrett and B. A. Robson, *"Nucleon exchange effects in ^{16}O - ^{16}O scattering"* submitted to *Nucl. Phys.* A.

NOTATION

In this thesis all vectors are written in a bold typeface e.g. $\mathbf{R}$ and $\mathbf{r}$. The corresponding lengths of these vectors are R and r, respectively. The only exceptions to this rule are the internal coordinates of clusters which are denoted ρ_i.

All matrices are written in italics e.g. B and its inverse B^{-1}. The matrix elements of these matrices are written B_{ij} and B^{-1}_{ij}, respectively.

ACKNOWLEDGEMENTS

It is a pleasure to thank my supervisor, Dr. Brian A. Robson, for allowing me to work with him and for his constant guidance and encouragement throughout this work. I also acknowledge my debt to him for devoting so much time and effort into critically reading the manuscript.

I would also like to thank Dr. Ross F. Barrett for the fruitful collaboration with him and the continued correspondence when he moved to Perth.

I am very grateful to Professor Kenneth J. LeCouteur for offering me an ANU scholarship to perform this work and for the hospitality extended to me by himself and his wife.

It is a pleasure to thank Mrs. Sally V. Lucas for patiently typing the manuscript, despite my handwriting, and to Mr. Richard J. Lucas for keeping her sane.

Finally, but not of least importance, I wish to thank my future wife, Cali, for helping and supporting me throughout this work.

ABSTRACT

Natural boundary condition methods and the generator coordinate method (GCM) are used to treat the scattering of composite particles. The procedure developed involves the concept of using the full GCM wave function as a *basis state*. The method is applied to α - α and ^{16}O - ^{16}O elastic scattering and the results are compared with other microscopic calculations.

Methods are developed to analyse the phase shifts in terms of the number of particles exchanged *between* the clusters. The no-particle exchange approximation is shown to be closely related to the Folding Model and results for all particle exchange approximations are presented and discussed. It is found that, contrary to earlier investigations, all particle exchange contributions act in the same direction and with roughly equal magnitudes. The discrepancy is shown to stem from inconsistent approximations in the earlier work.

The role of *forbidden* states is examined using the particle exchange analysis and the orthogonality condition model. It is found that the importance of such states depends on the effective two-body interaction employed.

Finally, some new approximation schemes for the exchange terms are considered and possible further calculations are suggested.

CONTENTS

CHAPTER 1

INTRODUCTION

The principle reason for the work is to show that the accurate and convergent natural boundary condition methods (Ahmad *et al* 1976 a, b) may be extended to a microscopic treatment of heavy-ion (HI) scattering. By microscopic it is meant that the ions are treated explicitly in terms of their constituent protons and neutrons and the interaction between the *ions* is determined by the forces between the *nucleons*. This is an increasingly important problem as more detailed and accurate HI reaction experiments are performed, which can not be accounted for satisfactorily using existing phenomenological and semi-phenomenological models. For example, many different models and mechanisms have been proposed (see e.g. Cindro 1977) for the so-called quasimolecular resonances and intermediate structure observed in HI reactions. This problem is only likely to be resolved by a microscopic calculation using realistic nuclear forces.

Clearly, such problems are formidable and are certainly not solved in this thesis. However, the goal of understanding HI reactions in terms of the detailed nuclear structure provides the impetus for this effort. In this thesis, an efficient and *properly convergent* method, derived from the well established and general R-matrix reaction theory is extended to the problem of HI scattering. An R-matrix method has already been developed (Baye *et al* 1977) which has shown that this approach is useful (Baye *et al* 1978).

The R-matrix methods also permit a detailed study of the effects of

the Pauli principle in microscopic calculations. Full antisymmetrisation of the total wave functions is very important but introduces many computational problems and therefore a good understanding is required so that approximations may be made.

Already in describing the problem the main assumption of nuclear physics has been made, namely that nuclei are composed of protons and neutrons, which are considered to be fundamental particles. Other general assumptions made are that *only* nucleons need to be considered (i.e. no mesons) and that all interactions may be represented by non-relativistic potentials. Furthermore, although 3-body forces may be important (Eisenberg and Greiner 1976), especially if the higher order forces significantly affect the structure (Robson 1979), they are ignored for simplicity and the nucleon-nucleon interaction is represented by a two-body effective potential. Finally it is assumed that in HI reactions, true three-body *breakup* of the compound system rarely occurs (Specht 1978) and for the range of energies and ions considered in the present work coulomb excitation is negligible.

Reaction theories may be classified into two groups: (i) *structural* (or *S-matrix*) *theories*, which are based on structural assumptions such as conservation of flux and time reversal invariance and (ii) *dynamical theories*, which use the detailed dynamics of the nuclear system to describe the interaction region. The S-matrix theories have been developed along formal lines (Eden 1966) and provide a useful prescription for parametrising nuclear resonances (e.g. McVoy 1971). However, these formulations may not be used as a tool for calculating reaction cross sections because they have no definite connection with the dynamic structure of the nuclei. On the other hand the dynamical theories are *based* on an assumed model of the interacting system so that the reaction data can be directly related to the nuclear structure.

The dynamical theories have been discussed comprehensively within a general formal framework (Lane and Robson 1966) based on the formulation due to Bloch (1957). Of these theories, the most widely known and extensively

used are those related to the *R*-matrix theory (Lane and Thomas 1958). The *R*-matrix theory is based on the intuitively appealing notion of dividing configuration space into an *internal region*, in which all nuclear reactions are assumed to occur, and an *external region*, where the nuclei interact only via the long-ranged coulomb force. The wave functions in the two regions are connected via the *R*-matrix, which contains all the reaction information necessary to calculate any observable quantities.

In the external region, the relative motion of the two ions may be described by specifying the wave number k and angular momentum quantum numbers L, M. The internal states of the nuclei are specified by a set of quantum numbers $\{\alpha\}$. If these internal states of the nuclei couple with the relative motion to form a system with total angular momentum J and projection M_J, then the set $\{L, J, M_J, \alpha\}$ defines a *channel*, which is a possible outcome of the nuclear reaction. The incoming nuclei constitute the *elastic channel*, residual products involving simple excitation of the ions are *inelastic channels* and *reaction channels* involve rearrangement of the nucleons. Only two-body breakup is considered so that the internal region is defined by a set of *matching radii*, $\{a_c\}$, which are the relative separations of the two nuclei at the surface of the internal region. In most of the work described in this thesis only single-channel elastic scattering is considered, but some results of a multichannel calculation are reported in chapter 7.

R-matrix theories are generally applicable to many reaction phenomena, particularly resonances (Lane 1967) and have been adapted to the theoretical study of nuclear reactions using several different methods (Nagarajan *et al* 1965, Lane and Robson 1969, Tobocman 1978, Chandler and Tobocman 1979). They have also been used to solve the composite particle problem (Horiuchi 1970, Baye and Heenen 1974b, 1977a, b).

These attempts to use *R*-matrix theory for the treatment of cluster

scattering have involved the use of the generator coordinate method (GCM). The GCM and the closely related resonating group method (RGM), which are discussed in chapter 3, both rely on the solution of an integral equation for a relative wave function, which is then matched to an asymptotic form. In the RGM this asymptotic form is the usual coulomb wave function and the matching is exact, but, at the cost of integral kernels which are difficult to evaluate. In the GCM, however, the corresponding kernels are relatively easily determined but the matching is to an unknown wave function in *generator coordinate space*. This problem has been overcome in the above mentioned *R*-matrix methods and also by several other authors (Mito and Kamimura 1976, Canto and Brink 1977, Nagata and Yamamoto 1977). All these methods involve an ansatz for the relative wave function and only use the GCM kernels in the internal region, so that no asymptotic GCM wave functions are required. In this thesis, the matching problem is overcome by using the GCM wave function as a *basis state*, so that any choice may be made for the GCM weight function (see §3.1). However, to optimise the calculation, the GCM weight function is chosen to give rise to scattering type wave functions.

Alternatives to these *R*-matrix methods for microscopic cluster scattering are the time-dependent Hartree-Fock (TDHF) method (Flocard *et al* 1978, Bonch *et al* 1978) and some classical models (Wilets *et al* 1978, Nunnelley and Thomas 1978). In each of these approaches, there are problems in relating the model description to experimental data, although some progress has been made recently in this respect for the TDHF (Sandhya Devi *et al* 1979). Moreover, TDHF calculations of heavy-ion scattering require huge computing resources while the classical methods cannot be expected to reproduce all features of the observed scattering. However, these methods do allow a visualisation of what is "happening" during a collision and so may help in deciding what features are required in any model of the interacting system.

Recent work has shown (Ahmad *et al* 1976a, b, Ahmad and Boccaccio 1978,

Barrett and Robson 1979) that, of all methods derived from the *R*-matrix theory, the *natural boundary condition* (NBC) methods converge fastest and uniformly with respect to the size of the basis. There are two NBC methods: (i) the *Barrett and Delsanto* (BD) method (Barrett and Delsanto 1974) derived from the eigenchannel method (Danos and Greiner 1966) and (ii) the *iterative R-matrix* (IRM) method (Ahmad *et al* 1976 a, b, Ahmad 1978a) derived more directly from *R*-matrix theory. These two methods have been shown to be equivalent but in this work the BD method has been utilised because it is more efficient for elastic scattering for which no iteration procedure is necessary.

The reason for devising another method of using the GCM kernels was to allow the properly convergent NBC methods to be employed in the calculation of cluster scattering. By choosing a method which has been shown to be applicable to the treatment of reactions, nuclear or otherwise (Barrett and Robson 1979), it was hoped that any method developed for elastic scattering may also be readily generalised to coupled-channels problems. Chapter 2 describes the BD method for elastic scattering and chapter 3 shows how the GCM may be used to define a suitable basis to solve the problem of composite particle scattering.

Also discussed in chapter 2 is the problem of defining an internal region for cluster scattering since asymptotically only a certain *fragmentation* of the compound system is observed but this may correspond to very many *partitions* of the identical nucleons into two clusters of the appropriate size. It is found that any partition may be used to define the internal region (Baye and Heenen 1974a) provided the wave function matched to the asymptotic form is renormalised to account for the neglected partitions. This problem has been solved in a very different way by the introduction of symmetrised coordinates (Pruess and Lichtner 1976). However, although this method may be very useful for a study of rearrangement collisions, it involves coordinate dependent masses and in general more

complicated equations. Symmetrised coordinates will not be considered further although any model developed using such coordinates may be readily employed in the NBC methods.

The effect of the Pauli principle upon the interaction between the ions is discussed in chapter 4. Also, it is shown how the results of GCM or RGM type calculations may be analysed in terms of the number of nucleons exchanged *between* the clusters. This, to the author's knowledge, has not been treated in a consistent manner before. Such detailed analysis also allows the study of the importance of any *forbidden states* and it is found that this depends on the particular choice of effective potential.

Chapters 5 and 6 describe the application of the methods described in chapters 2, 3 and 4 to α - α and ^{16}O - ^{16}O elastic scattering, respectively. All the results of these calculations are presented in the form of phase shifts which completely determine the scattering (Jackson 1970). Although it may be possible to calculate an energy dependent effective interaction between the ions, this is not attempted in the present work. However, the effect of the antisymmetrisation on such a potential is discussed. In both chapters 5 and 6, the necessary analytic tools are described, the general method of solution is discussed and an assessment of the accuracy and stability of the method is given.

A further discussion of all the results calculated in chapters 5 and 6 is given in chapter 7. This discussion is split into three parts: (i) the BD method applied to composite particle scattering, (ii) effects of the Pauli principle and (iii) particle exchange approximations in cluster scattering. Also some approximate methods are tested. Finally chapter 8 is a brief summary of the main results and conclusions of this work.

CHAPTER 2

NATURAL BOUNDARY CONDITION METHODS

§2.1 Introduction

Natural boundary condition (NBC) methods (Barrett and Delsanto 1974, Ahmad *et al* 1976 a, b, Barrett and Robson 1979) have been shown to be suitable methods for nuclear or atomic reaction calculations as discussed in chapter 1. Using these methods multichannel calculations have been performed and compared with other coupled channels formulations. It has been shown that the NBC methods are both efficient and accurate. This is very important for the study of heavy-ion reactions where ultimately many inelastic and reaction channels may need to be considered.

The NBC methods only require overlap and Hamiltonian matrix elements calculated over the internal region and it is *demanded* that all observable results depend only on the particular nuclear model employed and not on any parameters introduced by the reaction theory. In particular, results are not optimised by varying the matching radius; rather this is used as a test of the stability of the calculation.

There are two NBC methods which have been shown to be equivalent (Ahmad *et al* 1976 a, b, Barrett and Robson 1979): (i) the matrix diagonalisation or Barrett and Delsanto (BD) method and (ii) the iterative R-matrix (IRM) method. In the present calculations, the BD method had been used because it is more efficient when only elastic scattering is considered. In the multi-channel case the disparity between the methods is small and one method may be used as a check of the other. In this thesis only the

theory for the BD method with a non-orthogonal basis will be presented. The IRM method has recently been reviewed and compared with other R-matrix methods by Ahmad (1978 a, b) and Ahmad and Boccaccio (1978).

§2.2 Internal Region for Cluster Scattering

The NBC methods are based on R-matrix theory (Wigner and Eisenbud 1947, Lane and Thomas 1958) and divide the configuration space of the nuclei into two regions: (i) an internal region in which all nuclear interactions are assumed to occur and (ii) an external region in which the two nuclei are sufficiently separated so that any *nuclear* interaction is negligible compared with the long-ranged *coulomb* force.

To define an internal region for two composite particles a relative separation coordinate must be defined. Because the wave functions involved satisfy the Pauli principle, all nucleons are equivalent and it is possible to define C different coordinates of radial separation $r^{(k)}$. For two clusters of A_1 and A_2 nucleons, respectively

$$\left.\begin{aligned} C &= \frac{1}{1+\delta_{A_1A_2}} \times \frac{A!}{A_1!A_2!} , \\ A &= A_1+A_2 , \end{aligned}\right\} \qquad (2.2.1)$$

and

$$r^{(k)} = \frac{1}{A_1}\sum_{i=1}^{A_1} r_i - \frac{1}{A_2}\sum_{i=A_1+1}^{A} r_i , \qquad (2.2.2)$$

where r_i are the particle coordinates and different radial separations $r^{(k)}$ are found by making all C possible permutations of nucleons between the clusters.

The internal region is now defined as that region of configuration space for which $|r^{(k)}| < a$, for all k where a is known as the channel or matching radius.

In the internal region any choice of the relative coordinate $r^{(k)}$ must be equivalent to any other. Externally each of these choices can give rise to an asymptotic wave function, which in the cases considered here, are all identical to the elastic channel. In this way there are C possible *partitions* of the A nucleon system into the same fragmentation of two clusters of A_1 and A_2 nucleons, respectively. These partitions are indistinguishable experimentally from each other and form the elastic channel if the nuclei are in their ground states. Correct account of all possible partitions must be taken when matching the internal and external solutions.

The full wave function depends on the 3A spatial coordinates of the particles plus their spin-isospin projections and the evaluation of the matrix elements is required over the internal region. For the spatial integrations a set of *cluster coordinates* (Wildermuth and McClure 1966) is defined:

$$\left.\begin{aligned} r &= \frac{1}{A_1}\sum_{i=1}^{A_1} r_i - \frac{1}{A_2}\sum_{i=A_1+1}^{A} r_i \ , \\ R_{CM} &= \frac{1}{A}\sum_{i=1}^{A} r_i \ , \\ \rho_i &= r_i - R_{CM} - \frac{A_2}{A} r \quad i = 1,\ldots,A_1 \ , \\ \rho_i &= r_i - R_{CM} + \frac{A_1}{A} r \quad i = A_1+1,\ldots,A \ , \end{aligned}\right\} \qquad (2.2.3)$$

where r is the separation of the two clusters, R_{CM} the total centre-of-mass coordinate and ρ_i are the internal coordinates. The ρ_i are not all independent and satisfy the relations

$$\sum_{i=1}^{A_1} \rho_i = \sum_{i=A_1+1}^{A} \rho_i = 0 \ . \qquad (2.2.4)$$

Clearly there are C possible such choices of cluster coordinates. To calculate the matrix elements over the internal region, one such set of coordinates, say (2.2.3), is chosen and integrations are performed over the

complete space of all coordinates except for r which is restricted to the sphere $|r|<a$. A problem arises from the fact that for any specific choice of the relative coordinate, the internal region defined by $|r|<a$ will include parts of the external region of the (C-1) other partitions (Baye and Heenen 1974a). However, provided the channel radius a is large enough, the contributions from these regions will be negligible because they arise from terms in the wave functions involving Pauli exchange between the clusters and therefore have a finite range. It has been found that in the present calculations the value of a is large enough for this purpose if it satisfies the requirement that the nuclear interaction is negligible. This is due to the short-ranged nature of the single particle states.

Throughout this thesis matrix elements evaluated over the internal region are denoted by angular brackets. Thus for operator A

$$A_{ij} = \langle\Psi_i|A|\Psi_j\rangle = \int_{\text{all space}} d\tilde{\rho}_1 \ldots d\tilde{\rho}_A dR_{CM} d\Omega_r \int_0^a r^2 dr \Psi_i^* A \Psi_j \ , \qquad (2.2.5)$$

where the tilde indicates the additional integration over spin-isospin coordinates and it must be remembered that two of the A internal coordinates ρ_i are dependent {viz. eq. (2.2.4)}.

§2.3 Elastic Scattering Phase Shifts

In the external region, it is assumed that the nuclei only interact via the coulomb repulsion so that the angular momentum projected wave function must be of the form

$$\tilde{\psi}_L = \mathcal{A}\{(\exp(-i\delta_L) I_L(kr) - \exp(i\delta_L) O_L(kr)) r^{-1} Y_{LM}(\Omega_r) \phi_1 \phi_2\} \ , \qquad (2.3.1)$$

where $I_L(kr)$ and $O_L(kr)$ are incoming and outgoing coulomb waves with wave number k, respectively. The vector r is the relative separation coordinate, ϕ_1 and ϕ_2 are antisymmetrised internal wave functions of the two clusters, the tilde denotes asymptotic form and the parameter δ_L is the elastic

scattering phase shift for angular momentum L. The operator $\mathcal{A}$ antisymmetrises the wave function within the curly brackets with respect to exchange of nucleons between the two clusters and will be referred to as the *exchange operator*. The exchange terms are the (C-1) indistinguishable elastic channels arising from different partitions of the nucleons and asymptotically correspond to a renormalisation of the matrix elements by a factor C.

The phase shift δ_L is determined by matching the external solution $\tilde{\psi}_L$ to the internal solution at the surface $|r| = a$. From the logarithmic derivative b of the wave function $\tilde{\psi}_L$ at r = a, i.e.

$$b = \left\{ r \frac{d\tilde{\psi}_L/dr}{\tilde{\psi}_L} \right\}_{r=a} , \qquad (2.3.2)$$

it is possible to calculate the scattering phase shift δ_L if the kinetic energy of relative motion of the two clusters, and thus the wave number k, is known. The boundary condition b and wave number k are determined from the solution in the internal region and so using eqs. (2.3.1) and (2.3.2)

$$\tan(\delta_L) = - \left\{ \frac{bF_L(ka) - aF_L'(ka)}{bG_L(ka) - aG_L'(ka)} \right\}, \qquad (2.3.3)$$

where $F_L(z)$ and $G_L(z)$ are the regular and irregular coulomb functions and the prime denotes differentiation with respect to z.

§2.4 Bloch *L*-Operator and Natural Boundary Conditions

In any reaction theory, if there are open channels present, the kinetic energy operator is no longer hermitian. If an internal region is defined, it can be shown (Bloch 1957, Lane and Robson 1966) that hermiticity can be restored by adding a surface contribution to the kinetic energy. This contribution is called the Bloch *L*-operator and in the single channel case is

$$L(B) = \frac{h^2}{2\mu} \delta(r-a) \left\{ \frac{d}{dr} - \frac{B-1}{a} \right\} , \qquad (2.4.1)$$

where B is the boundary condition parameter and μ is the reduced mass of the system.

Using this operator, the Schrödinger equation in the internal region may be written in the form

$$(H + L(B) - E_i)\psi_i = L(B)\psi_i \ , \qquad (2.4.2)$$

where ψ_i is the eigenstate with eigenenergy E_i.

If the condition

$$L(B)\psi_i = 0 \qquad (2.4.3)$$

is satisfied then the quantity B is defined to be the *natural boundary condition* (n.b.c.) parameter for the wave function ψ_i and is in general energy dependent. When condition (2.4.3) is satisfied B = b.

Equation (2.4.3) has been shown (Ahmad and Boccaccio 1978) to define a minimal set of basis states given a particular model. In the multichannel case, iteration is required to find the n.b.c. parameters, B_c, for each channel c at each energy. However, for the single channel case no iteration is necessary and the calculation can be very fast numerically.

§2.5 BD Method for Elastic Scattering

The BD method has been reported in the literature (Barrett and Delsanto 1974, Ahmad *et al* 1976 a, b) in some detail for multichannel scattering and antisymmetrised wave functions (Barrett and Robson 1979). Here the BD method for only one channel, which is particularly simple but illustrates the main principles of the NBC methods, is described.

The full wave function ψ_i may be expanded in terms of a complete set of basis states ϕ_j. In the usual R-matrix formulations it is assumed that these basis states are the eigenfunctions of a known unperturbed Hamiltonian H_o. However this is not necessary and the basis states used in this thesis, because of the requirement of antisymmetry, are not even orthogonal. On

the other hand the basis states are required to satisfy the boundary conditions

$$L(B)\phi_j = 0 \tag{2.5.1}$$

The overlap matrix O has elements

$$O_{ij} = \langle\phi_i|\phi_j\rangle \ , \tag{2.5.2}$$

with the closure relation

$$1 = \sum_{ij} |\phi_i\rangle O^{-1}_{ij} \langle\phi_j| \ , \tag{2.5.3}$$

where O^{-1} is the inverse of O.

The total wave function is expanded in terms of this basis:

$$\psi_i = \sum_j a_{ij}\phi_j \ , \tag{2.5.4}$$

where

$$a_{ij} = \sum_k O^{-1}_{jk} \langle\phi_k|\psi_i\rangle \ . \tag{2.5.5}$$

Multiplying the Schrödinger eq. (2.4.2) for the state ψ_i on the left by ϕ_k and integrating over the internal region gives

$$\sum_j a_{ij}\langle\phi_k|H + L(B) - E_i|\phi_j\rangle = \langle\phi_k|L(B)|\psi_i\rangle \ , \tag{2.5.6}$$

where the fact that the summation and integration may be interchanged (Lane and Robson 1967) has been used. If the boundary condition parameter B is *natural*, eq. (2.5.6) reduces to the equation

$$\sum_j a_{ij}\langle\phi_k|H - E_i|\phi_j\rangle = 0 \ . \tag{2.5.7}$$

This matrix equation can easily be solved numerically to obtain the eigenvalues E_i and expansion coefficients a_{ij} in a truncated basis set $\{\phi_i; i\leq\mu\}$, where μ is the number of basis states. The number μ is determined by the convergence of the phase shifts in the energy region of interest.

Asymptotically the allowed values of the kinetic energy of separation, T_i, of the two clusters are given by

$$T_i = E_i - (B_1 + B_2), \tag{2.5.8}$$

where B_1 and B_2 are the binding energies of the two clusters. From the calculated values of T_i, corresponding to a given value of B, the wave number k in eq. (2.3.1) and hence the phase shift may be calculated using eq. (2.3.3). By letting B vary through the range + ∞ to - ∞ the phase shift δ_L may be obtained at all energies.

§2.6 Distant Levels Approximation

To solve the Schrödinger equation for a given system the infinite summation (2.5.4) is truncated to μ levels (basis states). Suppose that the eigenvalues and eigenvectors for this truncated basis have already been determined then the effect of introducing an extra level can be investigated.

Suppose that eq. (2.5.7) has been solved for a given set of basis states to obtain the eigenstates ψ_i (with eigenvalues E_i), which satisfy

$$\left.\begin{aligned} L(B)\psi_i &= 0 \ , \\ \sum_j a_{ij}\{H_{kj} - E_i O_{kj}\} &= 0, \\ \sum_{jj'} a_{ij} O_{jj'} a_{i'j'} &= \delta_{ii'} \ , \end{aligned}\right\} \qquad (2.6.1)$$

where the last equation is the orthogonality condition for the eigenstates ψ_i and H_{kj}, O_{kj}, are the Hamiltonian and overlap matrix elements for the basis $\{\phi_j\}$, respectively.

The same equation (2.5.7) can now be solved with a new basis comprised of the μ "old" eigenstates ψ_i plus an extra basis state ϕ_m. The "new" eigenstates $\bar{\psi}_i$ with eigenvalues $\bar{E}_i$ can be written

$$\bar{\psi}_i = \sum_{j=1}^{\mu} b_{ij}\psi_j + b_{im}\phi_m \ , \qquad (2.6.2)$$

and the secular equations for the expanded basis are

$$\sum_j b_{ij}\langle\psi_k|H-\bar{E}_i|\psi_j\rangle + b_{im}\langle\psi_k|H-\bar{E}_i|\phi_m\rangle = 0 \ , \qquad (2.6.3a)$$

$$\sum_j b_{ij}\langle\phi_m|H-\bar{E}_i|\psi_j\rangle + b_{im}\langle\phi_m|H-\bar{E}_i|\phi_m\rangle = 0. \qquad (2.6.3b)$$

Using eq. (2.6.1) and (2.6.3a) it is easy to show that

$$b_{ik}(E_k-\bar{E}_i) + b_{im}\langle\psi_k|H-\bar{E}_i|\phi_m\rangle = 0 \ , \qquad (2.6.4)$$

and substituting the value of b_{ik} given by this equation into eq. (2.6.3b) gives

$$H_{mm} - \bar{E}_i O_{mm} + \sum_j \frac{\omega_{mj}^2}{\bar{E}_i - E_j} = 0 \ , \qquad (2.6.5)$$

where

$$\left.\begin{aligned} H_{mm} &= \langle\phi_m|H|\phi_m\rangle, \ O_{mm} = \langle\phi_m|\phi_m\rangle \ , \\ \omega_{mj} &= \langle\phi_m|H-\bar{E}_i|\psi_j\rangle = \sum_{k=1}^{\mu} a_{jk}\langle\phi_m|H-\bar{E}_i|\phi_k\rangle \ . \end{aligned}\right\} \qquad (2.6.6)$$

To obtain eq. (2.6.5) it is necessary to use the fact that H is a hermitian operator since the basis states satisfy natural boundary conditions.

The effect of the additional state ϕ_m on the eigenvalues of the system can be visualised by solving eq. (2.6.5) graphically. The two functions

$$f_1(\bar{E}) = \sum_j \frac{\omega_{mj}^2}{(\bar{E} - E_j)} \qquad (2.6.7)$$

and

$$f_2(\bar{E}) = (\bar{E}O_{mm} - H_{mm}) \qquad (2.6.8)$$

are plotted in figure 2.1. The function $f_1(\bar{E})$ has simple poles at $\bar{E} = E_j$ and since ω_{mj}^2 is always positive, $f_1(\bar{E}) \to -\infty$ as $\bar{E}$ approaches E_j from below and $f_1(\bar{E}) \to +\infty$ as $\bar{E}$ approaches E_j from above. The function $f_2(\bar{E})$ is a straight line of positive slope (since $O_{mm} > 0$). The points of intersection of the two functions in figure 2.1 correspond to the new eigenvalues $\bar{E}_j$ of the system.

From figure 2.1 it is seen that a new eigenvalue $\bar{E}_j$ is always lower

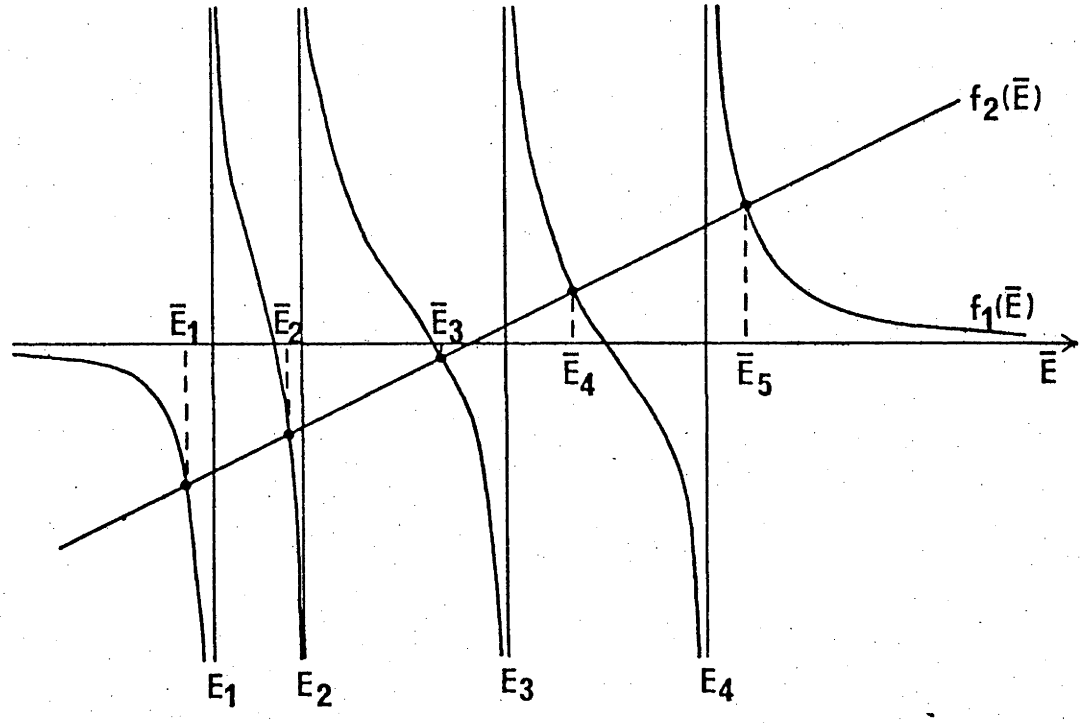

FIGURE 2.1 Hylleraas-Undheim theorem for nonorthogonal states. Graphical solution of eq. (2.6.8).

than the corresponding original eigenvalue E_i. Consequently, the calculated eigenvalues for any truncated basis set are always greater than the exact values of the system. This is essentially a graphical statement of the Hylleraas-Undheim theorem (Hylleraas and Undheim 1930, MacDonald 1933).

If it is assumed that ϕ_m is distant in energy and only has a very small effect so that $\bar{E}_i \simeq E_i$ then only one term in the sum (2.6.5) contributes significantly, namely j = i and eq. (2.6.5) reduces to

$$H_{mm} - \bar{E}_i O_{mm} + \frac{\omega_{mi}^2}{\bar{E}_i - E_i} = 0. \tag{2.6.9}$$

Rearrangement of this equation gives

$$\bar{E}_i = E_i - \frac{\omega_{mi}^2}{H_{mm} - \bar{E}_i O_{mm}} . \tag{2.6.10}$$

The second term on the right hand side of this equation is already of the order $\delta E_i = (E_i - \bar{E}_i) << E_i$ so that this term is given to a good approximation when $\bar{E}_i$ is replaced by the corresponding known eigenenergy E_i i.e.

$$\bar{E}_i \simeq E_i - \frac{\omega_{mi}^2}{H_{mm} - E_i O_{mm}} , \tag{2.6.11}$$

where the energy in the expression for ω_{mi} is now E_i. This is the approximate expression in the BD method for the new eigenvalue when a distant level is included.

The eigenfunctions are also slightly modified by the inclusion of this extra state. Substituting eq. (2.6.4) into eq. (2.6.2) gives

$$\left.\begin{aligned} \tilde{\psi}_i &= \sum_{j=1}^{\mu} \frac{b_{im}\omega_{jm}}{\bar{E}_i - E_j} \psi_j + b_{im}\phi_m , \\ &\simeq \frac{b_{im}\omega_{im}}{\bar{E}_i - E_i} \psi_i + b_{im}\phi_m \end{aligned}\right\} \tag{2.6.12}$$

and since the phase shifts are independent of the overall normalisation

eq. (2.6.11) may be written

$$\tilde{\psi}_i \simeq \psi_i + \bar{b}_{im}\phi_m \tag{2.6.13}$$

and the expansion coefficients a_{ij} are unchanged by the inclusion of ϕ_m.

Provided the state being treated approximately is considerably removed in energy from the region of interest, the effect on the energy eigenvalue E_i of the addition of successive such states is additive.

CHAPTER 3

GENERATOR COORDINATE METHOD WAVE FUNCTIONS

§3.1 Introduction

The generator coordinate method (GCM) was first proposed by Hill and Wheeler (1953) as a means of representing nuclear collective motion or modes of excitation, such as rotations and vibrations and at the same time retaining a microscopic wave function. These methods have been extensively reviewed recently (Wong 1975). The general principle is to devise a wave function $\phi(r_i;\alpha)$, where r_i are the particle coordinates and the parameters α describe the collective motion to be included, and then to construct a trial wave function or ansatz for the full wave function $\Psi(r_i)$ of the system. Specifically, one writes

$$\Psi(r_i) = \int d\alpha\ \phi(r_i;\alpha) f(\alpha) \ , \tag{3.1.1}$$

where the quantities α are called the *generator coordinates* and $f(\alpha)$ is the *generator coordinate weight function*. By introducing the Hamiltonian H, and using the variational principle

$$\delta E = \delta\left\{ \frac{\{\Psi|H|\Psi\}}{\{\Psi|\Psi\}} \right\} = 0 \tag{3.1.2}$$

to extremise the total energy E, an integral equation for the weight function is obtained (Griffin and Wheeler 1957):

$$\int d\alpha'\{H(\alpha,\alpha') - EO(\alpha,\alpha')\}\ f(\alpha') = 0 \tag{3.1.3}$$

This is the Hill-Wheeler (HW) integral equation and $H(\alpha,\alpha')$, $O(\alpha,\alpha')$

are the Hamiltonian (or energy) and overlap integral kernels, respectively. More explicitly

$$\left.\begin{aligned} H(\alpha,\alpha') &= \{\phi(r_i;\alpha)\,|H|\,\phi(r_i;\alpha')\}\ , \\ O(\alpha,\alpha') &= \{\phi(r_i;\alpha)\,|\,\phi(r_i;\alpha')\}\ , \end{aligned}\right\} \qquad (3.1.4)$$

where the integrations are performed over all space of the particle coordinates and are denoted by the curly brackets throughout this thesis.

The usual technique employed to solve eq. (3.1.3) is to discretise the integral by introducing a finite set of values $\{\alpha_i\}$, for the generator coordinates and to solve the matrix equation

$$\{H - E\,O\}\,f = 0\ , \qquad (3.1.5)$$

where $H_{ij} = H(\alpha_i\ ,\ \alpha_j)$, $O_{ij} = O(\alpha_i\ ,\ \alpha_j)$ and f is the set of values $\{f(\alpha_i)\}$. Matrix equations of this type are readily solved numerically.

The significant merit of the GCM and the closely related resonating group method (RGM) is that prior physical knowledge may be built into a truly microscopic model. In this way, specific forms of collective motion may be studied in a microscopic way without the need to include a huge number of basis states of, for example, the shell model. There has been much theoretical work on the interpretation of collective motion with the GCM formalism (Mihailovic and Rosina 1973, Wong 1975) and these methods have been successful in describing collective phenomena in various nuclei (Brink 1966, Mihailovic and Rosina 1973, Wong 1975, Wildermuth and Tang 1977). The GCM has also been applied to the problem of heavy-ion scattering (Baye 1976, Baye and Heenen 1976, 1977a, Canto 1977, Baye and Salmon 1979).

The practical difficulties of the GCM lie in the actual evaluation of the integral kernels because in general the basis states $\phi(r_i;\alpha_j)$, are non-orthogonal and the antisymmetrisation results in a large number of terms to be considered. Numerical calculation of the kernels involves the addition and subtraction of large terms which can cause serious errors. This has

been overcome recently by the use of techniques devised to calculate these kernels analytically (Tohsaki-Suzuki 1977, Baye and Heenen 1977b).

A second problem arising from the non-orthogonality of the basis states can occur if one or more of the eigenvalues of the overlap matrix is near zero, i.e. if the basis is nearly linearly dependent (Brink 1966). In this case the expansion

$$\Psi(r_i) = \sum_j \phi(r_i;\alpha_j)\ f(\alpha_j) \qquad (3.1.6)$$

is said to be ill conditioned. This problem has been considered in detail by Galetti and Toledo Piza (1978) who compare an exactly solvable model with numerical calculations and find that the numerical solution can appear to stabilise, which is a commonly used criterion for convergence, at the wrong eigenvalues.

A third difficulty arises when attempting to use the GCM to generate a scattering solution. If the generator coordinates $\{\alpha_i\}$, are distributed on a mesh, the weight function $f(\alpha_i)$ oscillates more violently as the points become closer together. Lumbroso (1974) has shown that this is due to the behaviour of the Fourier transform of $f(\alpha)$ which contains a quadratic exponential term so that the transform back to $f(\alpha)$ diverges at high frequency. This means that in any practical calculation the solution for $f(\alpha)$ does not converge as the mesh size is decreased and the results may be only *semi-convergent*. This is not true of all techniques used, however, and in fact the discretisation may be put on a secure foundation (Broeckhove and Deumens 1979).

In this work problems of the first kind are avoided by calculating all the kernels involved analytically. Problems of the second and third kind are avoided by introducing a linearly independent set of functions for $f(\alpha)$ to define a set of *basis states*, using eq. (3.1.1), rather than attempting to solve the HW equation.

In the next section these basis states are defined and their asymptotic form discussed. A discussion of how the matrix elements may be calculated appears in section 3. In section 4 the asymptotic form of the basis states is used to define a *direct potential* acting between the two nuclei. This is exactly equivalent to the RGM direct potential and it is shown how this interaction is related to the usual folded potential. Finally section 5 describes how the GCM kernels may be calculated.

§3.2 Basis States

For the problem of the scattering of two composite particles, a microscopic model for the interaction region is required, which must behave like two clusters asymptotically and yet look like a compound nucleus for large overlap. A suitable wave function is of the type proposed by Margenau (1941) for the α - α system, cast into the form of a GCM trial function by Biel (1957) and into its present form by Brink (1966).

For the two cluster problem the wave function is

$$\Psi(r_i) = \int dR \; \mathcal{A}\{\phi_1(\tfrac{A_2}{A}R)\phi_2(-\tfrac{A_1}{A}R)\}\; f(R) \qquad (3.2.1)$$

$$= \int dR \; \phi(R)\; f(R),$$

where $\phi_1(\frac{A_2}{A}R)$ is the wave function of cluster 1 containing A_1 nucleons with single particle states centred at $\frac{A_2}{A}R$, $\phi_2(-\frac{A_1}{A}R)$ is the wave function of cluster 2 containing A_2 nucleons centred at $-\frac{A_1}{A}R$, $A = A_1 + A_2$ and R is the generator coordinate.

So that the problems considered are reasonably tractable, the single particle states are chosen to be harmonic oscillator orbitals multiplied by spin-isospin wave function. Furthermore the internal states of the nuclei are assumed to be the lowest shell model configuration.

The method presented in this thesis uses the GCM wave function (3.2.1) to construct a set of basis states, Ψ_{iLM} , for the expansion of the total wave function ψ_{iLM}. An arbitrary choice can therefore be made for the generator coordinate weight function $f(R)$. However, to ensure a rapid convergence of the expansion of ψ_{iLM} , $f(R)$ is chosen so that the basis states have a suitable asymptotic form. The choice

$$f(R) = j_L(k_i R)\ Y_{LM}(\Omega_R) \tag{3.2.2}$$

has been made, where $j_L(z)$ is a spherical Bessel function and $Y_{LM}(\Omega)$ the usual spherical harmonic. The basis states are defined as

$$\Psi_{iLM} = \int dR \phi(R) j_L(k_i R) Y_{LM}(\Omega_R). \tag{3.2.3}$$

Because these states are fully antisymmetric, all choices of cluster coordinates are equivalent. Inserting such a set of coordinates into eq. (3.2.3) it can be shown (see appendix A) that the asymptotic form, i.e. $|r| \to \infty$, of Ψ_{iLM} is

$$\Psi_{iLM} = Z(R_{CM}) j_L(k_i r) Y_{LM}(\Omega_r) \tilde{\phi}_1 \tilde{\phi}_2 , \tag{3.2.4}$$

where $\tilde{\phi}_1$, $\tilde{\phi}_2$ are antisymmetric cluster wave functions depending only on internal coordinates, r is the radial separation and R_{CM} is the total centre-of-mass coordinate. This is the form of an angular momentum projected plane wave and is clearly a suitable basis to represent a scattered wave. To take the antisymmetrisation properly into account all C partitions must be included. This gives rise to C indistinguishable, non-overlapping (in the external region) elastic channels so that the external solution must be matched to the function $C\tilde{\psi}_{iLM}$, where ψ_{iLM} is the full wave function and the tilde denotes asymptotic form.

The BD method imposes the boundary conditions

$$L(B)\Psi_{iLM} = 0. \tag{3.2.5}$$

If the matching radius is sufficiently large then Ψ_{iLM} will have achieved its asymptotic form at $|r| = a$ and the boundary conditions (3.2.5) using eq. (2.4.1) imply

$$\left(\frac{k_i r \, j_L'(k_i r)}{j_L(k_i r)} \right)_{r = a} = B - 1. \tag{3.2.6}$$

Eq. (3.2.6) defines a set of wave numbers $\{k_i\}$ which defines the set of basis states to be used in the internal region.

The choice (3.2.2) of $f(R)$ automatically projects out states of good angular momentum (asymptotically) and because in the present work only systems of identical clusters are considered a parity projection is unnecessary.

§3.3 Matrix Elements

The BD method requires the calculation of the Hamiltonian and overlap matrices over the internal region. Using the basis states Ψ_{iLM} written in terms of one of the possible sets of cluster coordinates, these matrix elements may be calculated by integrating all coordinates over all space except the relative separation r, which is confined to a sphere of radius a. The Hamiltonian matrix elements are of the form

$$H_{ij} = \int_{|r|<a} dr \int dR_{CM} d\tilde{\rho}_i \Psi^*_{iLM} H \Psi_{jLM} \tag{3.3.1}$$

and similarly for O_{ij}. In the α - α scattering example of the present work, this procedure can be followed exactly leaving a single integral over the internal region (from o to a) for the radial separation r.

The different terms contributing to this integral may be separated into two groups. The first is comprised of all terms which survive asymptotically, i.e. as $r \to \infty$, and they are referred to as the *direct terms of the matrix element*. The second group is comprised of the remaining terms,

which have a finite range and tend to zero exponentially as $r \to \infty$. These finite ranged contributions arise from the Pauli exchange in the wave functions and are referred to as *exchange terms of the matrix elements*. On account of this finite range these contributions to the matrix elements may be calculated by extending the range of integration to over all space, i.e. $a \to \infty$. Consequently these exchange terms may be determined using the GCM kernels with the direct terms being treated separately. This has been tested explicitly in chapter 5.

Thus

$$H_{ij} = \int dR dR' \, f_i^*(R) f_j(R') H(R,R') - C \int_{|r|>a} dr (\Psi_{iLM} | H | \Psi_{jLM}) \qquad (3.3.2)$$

and similarly for the overlap matrix, where the round brackets indicate integration over all coordinates except r and $H(R,R')$ is the GCM energy kernel. The second integral in eq. (3.3.2) actually diverges but is cancelled by the divergent term in the first integral. In actual calculations only the exchange terms of $H(R,R')$ are included in the first integral and then the second integral becomes $+C \int_{|r|<a} dr (\Psi_{iLM} | H | \Psi_{jLM})$, which is finite. The factor C describes the C equivalent elastic channels arising asymptotically from the fully antisymmetric wave function.

In this way the exchange contributions to the matrix elements have been evaluated using the easier to calculate GCM kernels while the direct terms are calculated exactly in the internal region and therefore the wave function can be matched to the true asymptotic form. This means that the calculational problems of the RGM and the matching problems of the GCM have been circumvented.

§3.4 Direct and Folded Potentials

This section describes how the direct contribution of the effective

interaction to the matrix elements may be expressed in terms of a *direct potential* acting between the ions. It is then shown how this direct potential is related to the usual folded potential which is far simpler to calculate and may serve as a useful approximation. This is tested in chapter 7 for the ^{16}O - ^{16}O example.

In the calculations performed in this thesis, a two body effective potential has been used and this may be divided into three parts:

$$V = \sum_{i<j=1}^{A} v_{ij}^{N} = \sum_{i<j=1}^{A_1} v_{ij}^{N} + \sum_{i<j=A_1+1}^{A} v_{ij}^{N} + \sum_{i=1}^{A_2} \sum_{j=A_1+1}^{A} v_{ij}^{N} \qquad (3.4.1)$$

$$= V_1 + V_2 + V_{INT}.$$

The first and second terms, V_1 , V_2 , correspond to internal potential energies for each cluster (strictly not defined for $r < a$ because of anti-symmetrisation) and the third term, V_{INT} , is the interaction potential between the nuclei. Using this interaction term and the asymptotic form of the basis states, Ψ_{iLM} , a direct interaction potential, $V_D(r)$, may be defined:

$$V_D(r) = \{\tilde{\phi}_1\tilde{\phi}_2|V_{INT}|\tilde{\phi}_1\tilde{\phi}_2\}, \qquad (3.4.2)$$

where only integrals over internal coordinates are performed. The contribution of the direct terms to the matrix elements H_{ij} for this part of the nuclear interaction may be written as

$$c\int_{r<a} dr \int dR_{CM} |z(R_{CM})|^2 \chi_i^*(r) V_D(r) \chi_j(r), \qquad (3.4.3)$$

where $\chi_i(r)$ is defined in §3.2.

If exchange between the two nuclei is entirely ignored then the scattering is simply that due to the potential $V_D(r)$. The problem of elastic scattering from such a local potential is most easily solved by numerical integration of the Schrödinger equation from r = 0 to r = a and

then matching the wave function to the known asymptotic form. This is used as a test of the accuracy and convergence of the BD method.

In eq. (3.4.2) the wave functions $\tilde{\phi}_1$, $\tilde{\phi}_2$ depend on internal coordinates which are not all independent, viz. eq. (2.2.4). This makes the evaluation of the potential $V_D(r)$ rather tedious, especially in the ^{16}O - ^{16}O case. If the integration in eq. (3.4.2) is approximated by allowing integration over A *independent* coordinates, and one renormalises accordingly, then because ϕ_1 and ϕ_2 are Slater determinants

$$\langle\tilde{\phi}_1\tilde{\phi}_2|V_{INT}|\tilde{\phi}_1\tilde{\phi}_2\rangle = A_1A_2\langle\tilde{\phi}_1\tilde{\phi}_2|v_{1\,A_1+1}^{N}|\tilde{\phi}_1\tilde{\phi}_2\rangle \tag{3.4.4}$$

$$= \int dr_1 dr_2 \rho_1(r_1)\rho_2(r_2)\bar{v}(r_1-r_2+r),$$

where $\rho_1(r_1)$ and $\rho_2(r_2)$ are the single particle densities of the two clusters, respectively:

$$\left.\begin{aligned} \rho_1(r_1) &= A_1 \int dr_2 \ldots dr_{A_1}\, \tilde{\phi}_1^*\tilde{\phi}_1 \,, \\ \rho_2(r_1) &= A_2 \int dr_2 \ldots dr_{A_2} \tilde{\phi}_2^*\tilde{\phi}_2 \,. \end{aligned}\right\} \tag{3.4.5}$$

The bar over the potential in eq. (3.4.4) denotes averaging over spin and isospin coordinates.

Equation (3.4.4) is just the usual definition of the folded potential $V_F(r)$, and has been used extensively in the folding model (Satchler and Love 1979). In this thesis, several effective interactions have been employed. For α - α scattering, calculations using a Volkov force 1 (Volkov 1965) will be discussed in chapter 5 and in the ^{16}O - ^{16}O case results using a Volkov force 2 will be compared with those for the Brink and Boeker (1967) potential B_1 in chapter 6. The direct and folded potentials calculated using these forces in equations (3.4.2) and (3.4.4), respectively, are plotted in figures 3.1 and 3.2. The actual analytic form

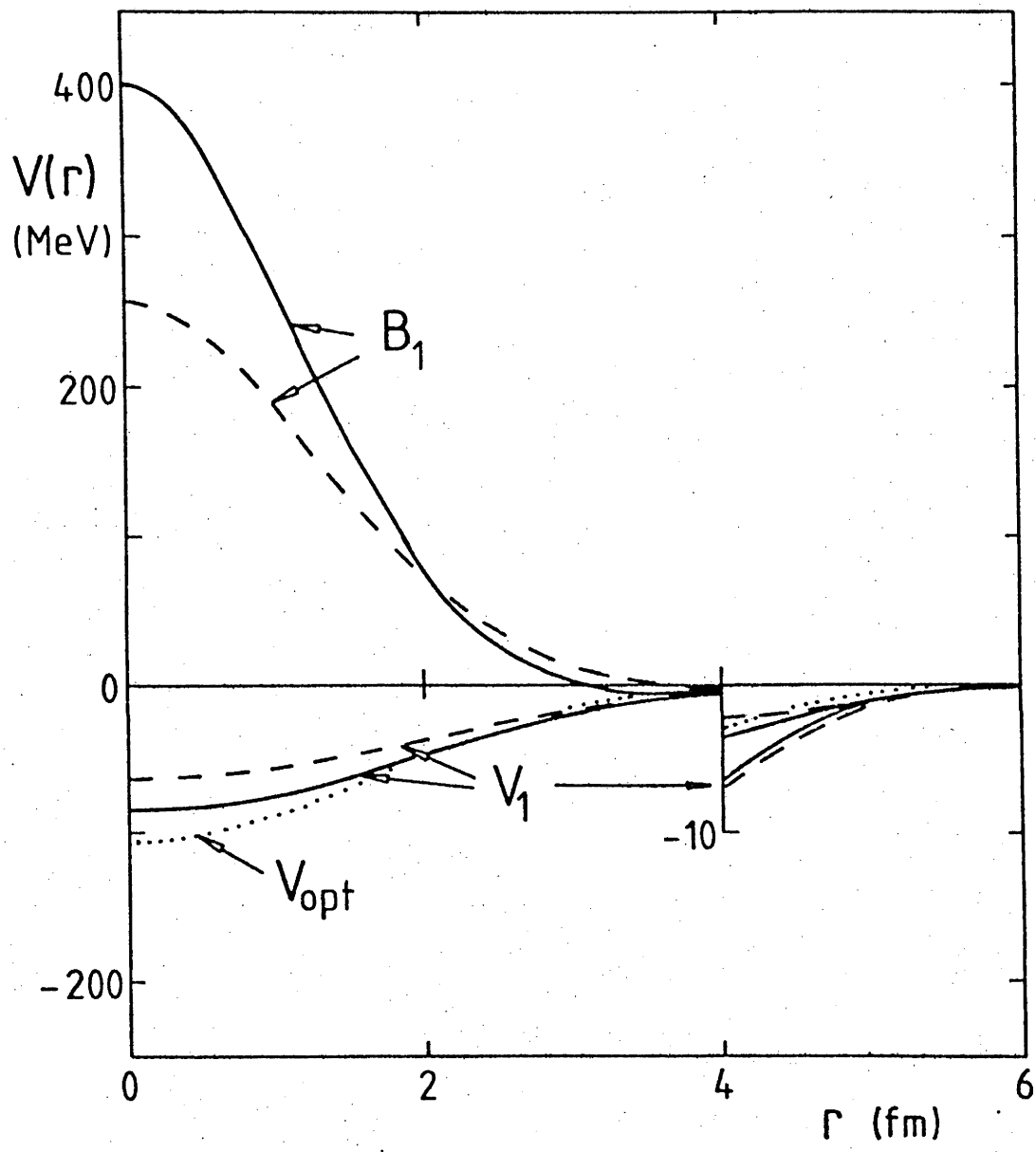

FIGURE 3.1 α - α direct and folded potentials. Solid curves are the direct potentials $V_D(r)$, dashed curves the folded potentials $V_F(r)$ and the dotted curve an optical potential (Afzal *et al* 1969). V_1 denotes potentials using the Volkov force 1, and B_1 denotes potentials using the Brink and Boeker force B_1.

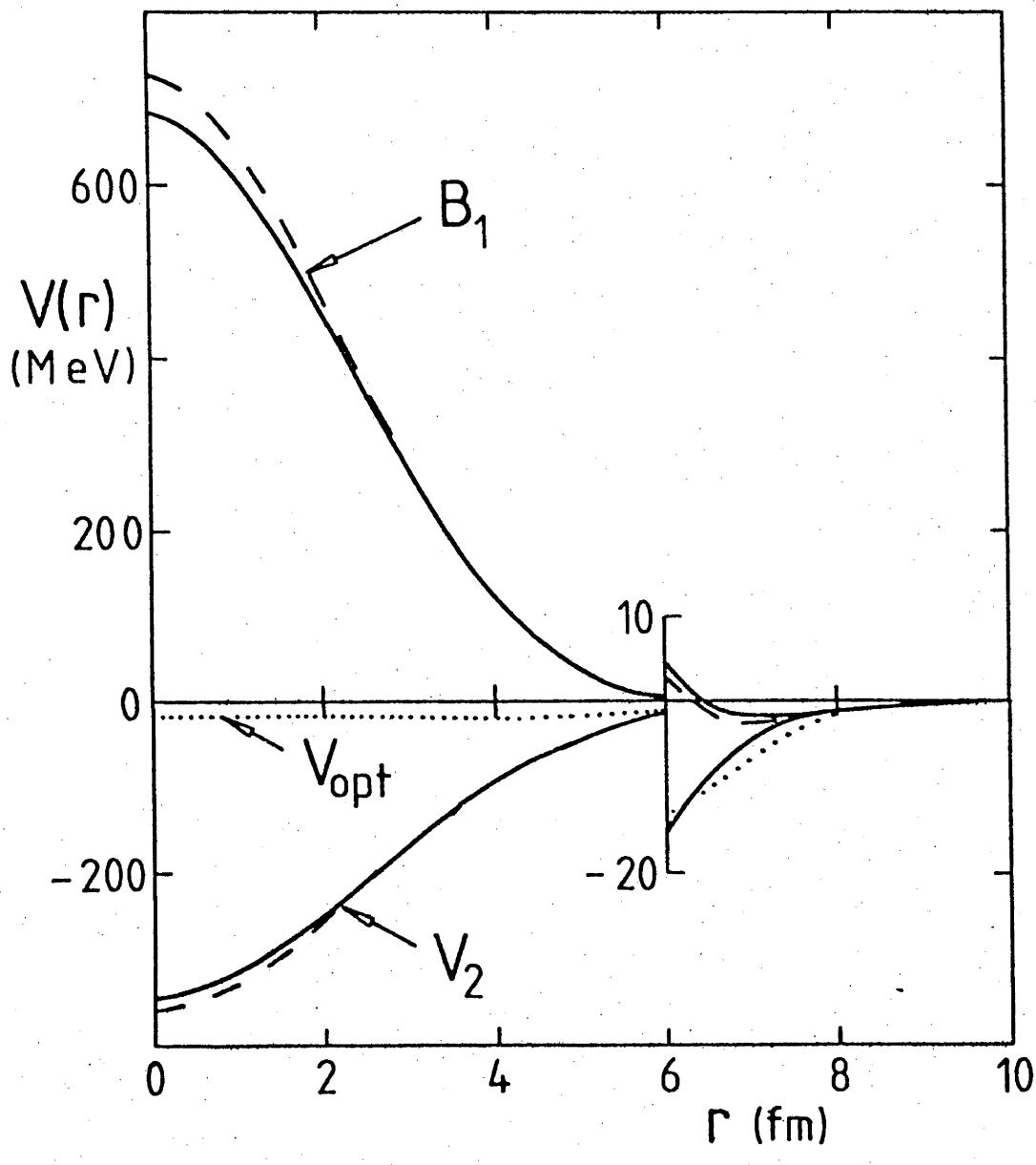

FIGURE 3.2 ^{16}O - ^{16}O direct and folded potentials. Same notation as fig. 3.1 but with a Volkov force 2 (V_2) and an optical potential from Gobbi *et al* (1973).

of $V_D(r)$ and $V_F(r)$ for both the α - α and ^{16}O - ^{16}O problems are detailed in appendix B along with all the potential parameters.

Also plotted for comparison are optical potentials which have been fitted to the elastic scattering data. The α - α potential is taken from Afzal *et al* (1969) and the ^{16}O - ^{16}O potential from Gobbi *et al* (1973).

Clearly the direct and folded potentials are slightly different. This will result in very similar phase shifts but resonances will be shifted accordingly as shown in chapter 7. Even more striking is the large difference between the potentials arising from the Volkov forces, which give very deep, attractive potential wells, and the Brink and Boeker force which gives a largely repulsive potential except near the surface. The dynamical result of this difference is discussed in chapters 6 and 7 but briefly, it is found that the Volkov potential supports many bound states and resonances whereas the B_1 potential does not, as would be expected. However, the two interactions are qualitatively phase equivalent on inclusion of exchange between the nuclei. This surprising result has been noted before (Weiguny 1977) and is discussed in detail in chapter 7.

§3.5 Calculation of the GCM kernels

Calculation of the GCM kernels is in principle straightforward although for larger clusters (> 4 nucleons) the analytic form required may involve very many terms. Only the outline of the method will be presented here since very detailed descriptions of the techniques have been given elsewhere (Horiuchi 1977, Tohsaki-Suzuki 1977).

The wave functions in the GCM kernels are

$$\phi(r_i;R) = \mathcal{A}\{\phi_1(+\frac{R}{2})\ \phi_1(-\frac{R}{2})\}\ , \qquad (3.5.1)$$

where now $\phi_1(+\frac{R}{2})$ is either the α-particle or ^{16}O ground state wave function

centred at $+\frac{R}{2}$. In either case the lowest shell model configuration is assumed with h.o. orbitals, i.e. $(1s)^4$ and $(1s)^4(1p)^{12}$, respectively.

The single particle states are a product of a h.o. wave function centred at $\pm\frac{R}{2}$ and one of four possible spin-isospin functions. For the α - α scattering problem, only one type of spatial state (1s - orbital) is involved while in the ^{16}O - ^{16}O wave function, there are four spatial states (a 1s-orbital and three 1p-orbitals). If the spin-isospin functions are written τ_1 , ..., τ_4 then the α - α wave function is

$$\phi(r_i;R) = \mathcal{A}\{\psi_1(r_1)\tau_1(1)\psi_1(r_2)\tau_2(2)\ldots\psi_1(r_4)\tau_4(4)\psi_2(r_5)\tau_1(5)\ldots \ldots\psi_2(r_8)\tau_4(8)\} \qquad (3.5.2)$$

where ψ_1 and ψ_2 denote the 1s-states centred at $\frac{1}{2}R$ and $-\frac{1}{2}R$, respectively. Similarly, the wave function for ^{16}O - ^{16}O scattering can be written as a product of 32 single-particle states with wave functions ψ_i (i=1,2,3,4) and ψ_j (j=5,6,7,8) denoting the 1s- and 1p- states centred at $\frac{1}{2}R$ and $-\frac{1}{2}R$, respectively.

The Hamiltonian is of the form

$$H = \frac{-\hbar^2}{2m}\sum_i \nabla_i^2 - \frac{3}{4}\hbar\omega + \sum_{i<j}(v_{ij}^N + v_{ij}^C) \qquad (3.5.3)$$

where the first term is the kinetic energy operator, the second term is the centre-of-mass energy and the third term represents the nuclear and coulomb interactions. For simplicity and to enable comparison with other methods, a central potential is adopted of the general form

$$v_{ij}^N = u(|r_i - r_j|)(w + bP_\sigma - hP_\tau + mP_M), \qquad (3.5.4)$$

where w, b, h and m are the usual Wigner, Bartlett, Heisenberg and Majorana exchange components, respectively. Since the wave functions for the α and ^{16}O nuclei have a special spin-isospin symmetry, namely S = T = 0, the integrations over spin and isospin variables may be performed explicitly

(Brink 1966) giving

$$O(R,R') = |\det B|^4 \tag{3.5.5}$$

and

$$H(R,R') = O(R,R')\Big\{4 \sum_{i,j} \{\psi_i|\frac{-\hbar^2}{2m}\nabla_j^2|\psi_j'\}B^{-1}_{ji} - \frac{3}{4}\hbar\omega$$

$$+ \sum_{ijkL} \{\psi_i\psi_j|u(r_{kL})|\psi_k'\psi_L'\}\{X_d B^{-1}_{ki}B^{-1}_{Lj} + X_e B^{-1}_{kj}B^{-1}_{Li}\}$$

$$+ \sum_{ijkL} \{\psi_i\psi_j|\frac{e^2}{r_{kL}}|\psi_k'\psi_L'\}\{2B^{-1}_{ki}B^{-1}_{Lj} - B^{-1}_{kj}B^{-1}_{Li}\}\Big\}\ , \tag{3.5.6}$$

where the matrix B has elements

$$B_{ij} = \{\psi_i|\psi_j'\} \tag{3.5.7}$$

and the prime denotes that the single particle state is centred at $\pm\frac{R'}{2}$.

In eq. (3.5.6) the ranges of summation of the indices i, j, k, L are the values 1 and 2 for the α - α system and the values 1, 2, ..., 8 for the ^{16}O - ^{16}O system. Also

$$\left.\begin{aligned} X_d &= 8w + 4b - 4h - 2m\ , \\ X_e &= 8m + 4h - 4b - 2w \end{aligned}\right\} \tag{3.5.8}$$

and B^{-1} is the inverse of B.

The GCM kernels for the ^{16}O - ^{16}O scattering have very many terms ($\sim 10^4$) and so algebraic computer techniques are essential. This problem has been solved in various ways (Baye and Heenen 1977, Tohsaki-Suzuki 1977). In the present work, the matrices B and B^{-1} are evaluated by hand and used, along with the required matrix elements in eq. (3.5.6), as input to a computer program which uses the symbolic code "REDUCE" (Hearn 1973) to calculate $O(R,R')$ and $H(R,R')$. For subsequent calculations, the kernels are stored in the form of coefficients of terms which are of the general form

$$Z(R,R') = d \exp\{-\nu(aR^2 + bR'^2)\}$$

$$\times \begin{cases} \text{Cosh}(c\nu R.R')(\nu R.R')^i (\nu R^2)^j (\nu R'^2)^k & i \text{ even}, \\ \text{Sinh}(c\nu R.R')(\nu R.R')^i (\nu R^2)^j (\nu R'^2)^k & i \text{ odd}. \end{cases} \qquad (3.5.9)$$

In appendix E the kernels for the α - α case are written down explicitly as an example. The matrices B, B^{-1} and the various one- and two-body matrix elements required for the ^{16}O - ^{16}O example are given in appendix F. Horiuchi (1977) has reviewed and discussed in detail all the various terms involved. The methods for calculating the GCM kernels for clusters with different oscillator parameters are given by Tohsaki-Suzuki (1977).

CHAPTER 4

ANTISYMMETRISATION

§4.1 Introduction

In any exact microscopic calculation involving a number of identical fermions the full wave function must satisfy the Pauli principle and be antisymmetric with respect to interchange of *any* two fermions. This full antisymmetrisation can significantly affect the results of a scattering calculation and may even dominate at certain energies. Of particular interest and importance are those effects arising from Pauli exchange *between* the clusters as these terms cause most of the difficulties in the calculation of the matrix elements and have been subject to many approximations.

The principle consequence of the antisymmetrisation is the Pauli distortion of the kinetic energy terms which refers to the fact that, due to blocking of intrinsic states of the compound system, the kinetic energy of the system increases. This manifests itself as an energy barrier over and above that due to compression of the nuclei. For example if two alpha particles were allowed to remain in their ground states with a relative separation of zero then there would be eight identical fermions in a (1s) level centred at the same point which is clearly forbidden by the Pauli principle. It can be shown (Brink 1965, Wildermuth and McClure 1966) that

if $R \rightarrow 0$ in eq. (3.5.1) then four of the nucleons are forced into the (1p) level and the Pauli principle can be satisfied.

The result of this blocking and promotion to higher levels is to make the effective potential between the two ions much shallower than that predicted by the simple folding model and may even give rise to a repulsive core. This is amply supported by many microscopic calculations of effective ion-ion interactions (Fliessbach 1971, Reidermeister 1972, Brink and Stancu 1975, Stancu and Brink 1976, Goritz and Mosel 1976, Zint and Mosel 1976, Zint 1977). These calculations are all microscopic, include full anti-symmetrisation and define the real part of the effective potential at separation R to be the total energy at separation R minus the total energy at ∞. These potentials agree qualitatively with optical potentials fitted to experimental data and show that the antisymmetrisation is very important.

The Pauli exchange is intrinsically non-local and this makes any effective nucleus-nucleus potential energy dependent. This problem was addressed microscopically by Fliessbach (1971), who finds that for higher energies the potential is deeper, i.e. more attractive, which is in agreement with experiment (Maher *et al* 1969) although the magnitude of the dependence found by Fliessbach is slightly smaller.

Another important consequence of the Pauli principle is a parity or an odd-even angular momentum dependence of the ion-ion interaction (LeMere *et al* 1979, Baye *et al* 1977, Zint 1977). This is not to be confused with an L-dependence of the *imaginary* part of the optical potential which is due to the low density of states of high spin at any particular energy because of

the proximity of the yrast level (Hodgson 1978). The parity dependence discussed here is due to the longer-ranged exchange terms of the GCM kernels cancelling or reinforcing the direct term depending on the L-value or parity of the relative wave function and hence is percieved as an L-dependence of the real part of the optical potential. The *identification* of these longer-ranged terms (LeMere *et al* 1979) as solely the core exchange contribution is incorrect (see §4.3) although the *conclusion* that L-dependence can arise is correct. In the special case of identical particles the L-dependence is absolute in that for odd angular momenta the terms cancel entirely. Optical potentials (Dehnhard *et al* 1978) with an L-dependent *real part* can give rise to the large back angle scattering observed recently in heavy-ion scattering (Barrette *et al* 1978).

Finally for wave functions of the form used here, with nuclei in their ground states asymptotically, there are certain relative motion states which are expressly forbidden by the Pauli principle. In these cases with harmonic oscillator (h.o.) single particle states all with the same range parameter, the forbidden relative motion wave functions are also h.o. states such that $2n + L < N_0$, where N_0 is determined by the lowest configuration possible in the compound system with the structure of eq. (3.5.1). When solving the scattering problem these null (sometimes referred to as redundant or superfluous) states can appear at any energy (Weiguny 1977) but usually at very large energies due to numerical inaccuracies. The solution of the scattering problem with only direct or folded potentials (§3.4) may involve bound states with quantum numbers corresponding to these forbidden states. Although these bound states will not be identical, they may be very close (in radial form) to the redundant h.o. orbitals in which case the inclusion of full

antisymmetrisation projects these states to very high energies. In this way bound states or resonances which may occur in the scattering from a folded potential will not occur if the problem is solved with full antisymmetrisation and care must be taken in any approximations to the Pauli exchange to ensure that such nearly forbidden states are not included in the solution. Moreover, the phase shifts at zero energy determined using Levinson's theorem (see §6.2) should include these redundant solutions as well as any true bound states (Englefield and Shoukry 1974, Weiguny 1977).

In this thesis no effective ion-ion potentials are calculated; however the various effects mentioned above are discussed in terms of the phase shifts which completely determine the scattering. In the next section the forbidden or superfluous states (Friedrich 1974) are studied and by using the orthogonality condition model (OCM) in its original interpretation (Saito 1969, Gridnev *et al* 1979), the importance of projecting out these states is investigated.In §4.3 that part of the antisymmetriser which interchanges nuclions between different clusters, hereafter referred to as the *exchange operator*, is studied in detail and the last two sections show how the 1-, 2-, ..., n- particle exchange approximations to the matrix elements are derived for the α-α and ^{16}O-^{16}O cases, respectively.

§4.2 Forbidden States

The forbidden states mentioned in §4.1 are relative motion states for which the total wave function is exactly zero when fully antisymmetric and are completely different to spurious centre-of-mass motion states which can exist after antisymmetrisation. In this work h.o. single particle orbitals with equal oscillator parameters have been used so that the total centre-of-

mass may be factorised out of the wave function thereby eliminating any possibility of c.m. excitations.

In terms of h.o. wave functions it is easy to determine which relative motion states are prohibited. Suppose the full wave function is of the form:

$$\Psi(R_{CM},r,\rho_i) = z(R_{CM})\chi(r)\Phi_1(\rho_i)\Phi_2(\rho_i), \qquad (4.2.1)$$

where R_{CM} is the total centre-of-mass coordinate, r is the distance between the centres-of-mass of the two clusters of A_1 and A_2 nucleons, respectively, with internal coordinates ρ_i. If all the single particle states in $\Phi_1(\rho_i)$ and $\Phi_1(\rho_i)$ are h.o. orbitals (with the same oscillator parameter ν) in their lowest configuration with no holes, and $z(R_{CM})$ and $\chi(r)$ are (1s) h.o. states (with oscillator parameters $(A_1+A_2)\nu$ and $\frac{A_1A_2}{A_1+A_2}\nu$, respectively) then it is well known that the resulting wave function has $2A_1$ (if $A_1 \leq A_2$) particles in the lowest A_1 levels and is therefore forbidden by the Pauli principle. In terms of Slater determinants certain columns would be exactly equal and thus the determinant identically zero.

These null states therefore arise from an attempt to put more than one fermion in each state. The number of redundant states is calculated using the requirement that the minimum number of oscillator quanta required in the compound system must be less than or equal to the total number in the scattering system.

Let us consider the α-α case as a simple example. In the compound system, ^{8}Be, the lowest allowed configuration is $(1s)^4(1p)^4$ with a total number of quanta of 4 (not including the 3/4 $\hbar\omega$ per particle). The α-α scattering system has a total of 0 quanta from the two α-particles and $(2n + L)$ quanta from the relative motion, where n and L are radial and angular momentum quantum numbers, respectively, therefore

$$2n + L \geq 4. \qquad (4.2.2)$$

For L = 0 the inequality (4.2.2) is not satisfied for n = 0,1 and thus there are two forbidden states, namely the 0s and 1s h.o. orbitals. For L = 2 the inequality (4.2.2) is violated for n = 0 and consequently only the 1d state is forbidden. For $L \geq 4$ relation (4.2.2) is satisfied for all n and there are no redundant states.

In the ^{16}O-^{16}O example the minimum number of quanta (N_0) in the compound system, ^{32}S, which must be of the form of eq. (3.5.1) is 48 corresponding to the configuration $(1s)^4\ (1p)^{12}\ (2s;1d)^{12}(2p;1f)^4$. In the scattering system each ^{16}O nucleus contributes 12 quanta therefore in this case

$$2n + L \geq 24.$$

Thus for all angular momenta $L < 24$ there exist forbidden states with a maximum number of 12 for L = 0. Bound or quasi-bound (forming sharp resonances) states with quantum numbers, n, L, *in the internal region* such that $2n + L < N_0$ will be referred to as states with forbidden quantum numbers. Although these states will not be exactly prohibited they may be very close to the corresponding h.o. wave function and so on antisymmetrisation will be projected to high energies. In the actual solution of eq. (2.5.7) for the eigenenergies these states appear as very large ($>10^5$) positive or negative eigenvalues. This is due to small numerical inaccuracies causing large changes to the nearly null states.

If particle exchange is ignored (e.g. the simple folding model) then these nearly forbidden states may be found either as bound states or will appear in the phases shifts as resonances which are removed by antisymmetrisation. Such spurious resonances can occur (see chapter 7).

Just how these prohibited states affect the scattering phase shifts if of interest for any approximation scheme (Bagchi *et al* 1980) and in fact the original OCM (Saito 1969) was based on the idea that the main effect of the particle exchange is to project out these states. More recent versions

(Saito 1977, Buck *et al* 1977) of the OCM also include an effective local potential to partially account for the non-local parts of the interaction (due to antisymmetrisation). To test the result of *just* forcing the solution to be orthogonal to the forbidden states, a projection operator Λ is defined:

$$\Lambda = \sum_k |n_k><n_k| , \tag{4.2.3}$$

where $|n_k>$ are the forbidden relative motion h.o. states. Using only the direct terms (i.e. $V_D(r)$), eq. (2.5.7) is solved subject to the orthogonality condition (OC)

$$\Lambda|\psi_i> = 0. \tag{4.2.4}$$

This condition is automatically satisfied if instead of eq. (2.5.7) the secular equation

$$\sum_j a_{ij}\{<\phi_k|(1-\Lambda)H(1-\Lambda)|\phi_j> - E_i<\phi_k|(1-\Lambda)^2|\phi_j>\} = 0 \tag{4.2.5}$$

is solved. Since Λ is a projection operator

$$(1-\Lambda)^2 \equiv (1-\Lambda) \tag{4.2.6}$$

and

$$O'_{ij} = O_{ij} - \sum_k <\phi_i|n_k><n_k|\phi_j> , \tag{4.2.7}$$

where

$$O_{ij} = <\phi_i|\phi_i> . \tag{4.2.8}$$

Similarly for the Hamiltonian matrix,

$$H'_{ij} = <\phi_i|H|\phi_j> - <\phi_i|\Lambda H + H\Lambda|\phi_j> + <\phi_i|\Lambda H\Lambda|\phi_i> \tag{4.2.9}$$

$$= H_{ij} - \sum_k \{<\phi_i|n_k><n_k|H|\phi_i> + <\phi_i|H|n_k><n_k|\phi_i>\}$$

$$+ \sum_{k,k'} <\phi_i|n_k><n_k|Hn_{k'}><n_{k'}|\phi_j>,$$

where

$$H_{ij} = <\phi_i|H|\phi_i> . \tag{4.2.10}$$

Using these formulae for the new matrices H' and O' it is straightforward to solve the direct potential problem and to satisfy the OC, eq. (4.2.4). The results for the α - α case are given in chapter 5 and are discussed further in chapter 7. The results agree with the general result (Englefield and Shoukry 1974) that the phase shift is increased by the OC.

§4.3 Particle Exchange Approximations

In this thesis a distinction has been made between *antisymmetrisation* which antisymmetrises the wave function with respect to interchange of any two particles and *exchange* which is with respect to the interchange of particles between clusters.

The antisymmetriser, $\mathcal{A}$, may be factorised into three components, one part, $\mathcal{A}'$, the exchange operator, which permutes particles located in different clusters and two others $\mathcal{A}_1, \mathcal{A}_2$ which act only on particles within clusters 1 and 2 respectively:

$$\psi_i = \left(\frac{A_1!A_2!}{A!}\right)^{\frac{1}{2}} \mathcal{A}'\mathcal{A}_1\mathcal{A}_2\overline{\psi}_i, \tag{4.3.1}$$

where the bar denotes that the wave function $\overline{\psi}_i$ is a simple product wave function and the numerical factor reflects the normalisation of $\mathcal{A}_1, \mathcal{A}_2$ and the original $\mathcal{A}$.

The exchange operator, $\mathcal{A}'$, may be split further into a sum of terms:

$$\mathcal{A}' = A_0 + A_1 + \ldots + A_N, \tag{4.3.2}$$

where A_n performs all possible n-particle exchanges of nucleons between the nuclei and N is the minimum of A_1 and A_2. In this way the A! terms of $\mathcal{A}$ are divided into (N + 1) groups of the general form $A_n\mathcal{A}_1\mathcal{A}_2$ and the n-particle exchange approximation to the wave function may be defined:

$$\psi_i^{(n)} = \sum_{k=0}^{n} A_k\mathcal{A}_1\mathcal{A}_2\overline{\psi}_i. \tag{4.3.3}$$

Any operator, symmetric in the particle coordinates, will commute with and also with any of the A! terms of $\mathcal{A}$, since these are merely permutation operators which by definition leave a symmetric operator unchanged. Also any one of the permutation operators, and hence $\mathcal{A}$ itself, is hermitean because, in any matrix element, the particle coordinates are dummy variables and may be relabelled. If P is such a permutation operator then

$$\langle P\bar{\psi}_i | H | \bar{\psi}_j \rangle = \langle \bar{\psi}_i | H | P\bar{\psi}_j \rangle. \tag{4.3.4}$$

The antisymmetriser $\mathcal{A}$ performs all possible permutations of the A particles in such a way that any odd (even) permutation gives rise to a minus (plus) sign. Thus

$$(-1)^p P\mathcal{A}\bar{\psi}_i = \mathcal{A}\bar{\psi}_i. \tag{4.3.5}$$

$$\langle \mathcal{A}\bar{\psi}_i | H | \mathcal{A}\bar{\psi}_j \rangle = \sqrt{A!}\langle \bar{\psi}_i | H | \mathcal{A}\bar{\psi}_j \rangle \tag{4.3.6}$$

remembering that $\mathcal{A}$ contains a factor $(A!)^{-\frac{1}{2}}$. Consequently if $\bar{\psi}_i$ is normalised then so is $\mathcal{A}\bar{\psi}_i$ provided the single particle states are orthogonal. Equation (4.3.6) is the well known result that is is only necessary to antisymmetrise one state vector of the matrix element.

To study in detail the consequences of particle exchange, the expansions (4.3.1) and (4.3.2) are used in the Hamiltonian or overlap GCM kernels

$$\begin{aligned} H(R,R') &= \{\mathcal{A}\bar{\psi}(R) | H | \mathcal{A}\bar{\psi}(R')\} \\ &= \sqrt{A!}\{\bar{\psi}(R) | H | \mathcal{A}\bar{\psi}(R')\} \\ &= \sqrt{A_1!A_2!}\ \{\bar{\psi}(R) | H | (A_0+A_1+\ldots A_N)\mathcal{A}_1\mathcal{A}_2\ \bar{\psi}(R')\}. \end{aligned} \tag{4.3.7}$$

Here and for the rest of this section the integrations for the matrix elements are over all space and is denoted by curly brackets.

Each of these sets of terms corresponding to the operator $A_n\mathcal{A}_1\mathcal{A}_2$ may be identified in the full expression for the Hamiltonian (or overlap) kernels because they have a characteristic exponential form and range. The

terms from the A_0, A_1, ..., A_N exchange operators have been identified (Horiuchi 1977, LeMere *et al* 1979) as the 0-, 1-, 2-, ..., N- particle exchange contributions to the GCM kernels respectively and define the n-particle exchange approximation

$$H^{(n)}(R,R') = \sqrt{A_1!A_2!}\{\overline{\psi}(R)|H|(A_0+A_1+\ldots+A_n)\mathcal{A}_1\mathcal{A}_2\overline{\psi}(R')\} \tag{4.3.8}$$

$$= \sum_{k=0}^{n} \overline{H}^{(k)}(R,R'),$$

where

$$\overline{H}^{(k)}(R,R') = \sqrt{A_1!A_2!}\{\overline{\psi}(R)|H|A_k\mathcal{A}_1\mathcal{A}_2\overline{\psi}(R')\} \tag{4.3.9}$$

and similarly for $O^{(n)}(R,R')$.

This identification of contributions to the GCM kernels is incorrect and the true n-particle exchange approximation is not given by eq. (4.3.8). The mistake arises because the truncated operator $(A_0+A_1+\ldots+A_n)$ must be taken into both state vectors of the matrix elements

$$H^{(n)}(R,R') = \{\psi^{(n)}(R)|H|\psi^{(n)}(R')\} \tag{4.3.10}$$

$$= \frac{\sqrt{A_1!A_2!}}{C}\{\overline{\psi}(R)|H|(A_0+A_1+\ldots+A_n)^2\mathcal{A}_1\mathcal{A}_2\overline{\psi}(R)\},$$

where C is defined by eq. (2.2.1), and it is *not true* in general (except n = 0, N) to write

$$(A_0+A_1+\ldots+A_n)^2\overline{\psi}_i \propto (A_0+A_1+\ldots+A_n)\overline{\psi}_i. \tag{4.3.11}$$

That eq. (4.3.8) is incorrect and in fact may give rise to non-physical effects is most easily demonstrated by calculating diagonal overlap matrix elements for different particle exchange approximations using the definitions (4.3.8) and (4.3.10). The approximate wave functions $\psi_i^{(n)}$ are still vectors in Hilbert space and must have positive norms (i.e. diagonal overlap matrix elements). Figure 4.1 shows this is not the case if the n-particle exchange approximation is defined by eq. (4.3.8). Plotted are the ratios of corresponding diagonal elements for $^{16}O - ^{16}O$ wave functions with the numerator defined by eq. (4.3.8). The norms defined by eq. (4.3.10) are all positive

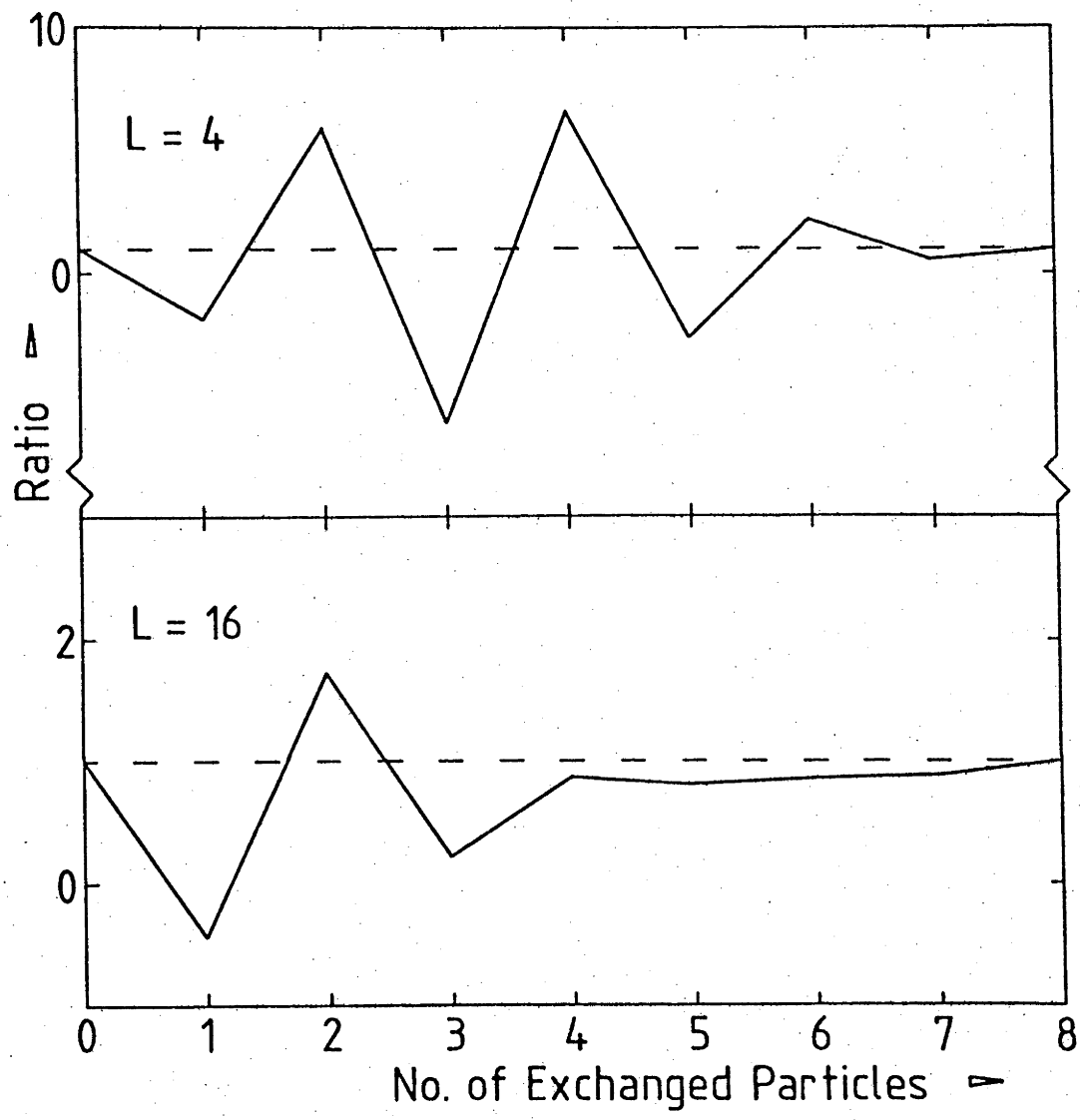

FIGURE 4.1 The ratio $O_{ii}^{(n)*}/O_{ii}^{(n)}$, where $O_{ii}^{(n)*}$ and $O_{ii}^{(n)}$ are diagonal overlap matrix elements calculated using eqs. (4.3.8) and (4.3.10) respectively. The L-values are marked and i = 4 and 14 for L = 4 and 16 respectively. Actual values of $O_{ii}^{(n)}$ are all positive and decrease monotonically from n = 0 to n = 8.

and decrease monotonically whereas the norms defined by eq. (4.3.8) oscillate wildly and alternate in sign leading to complex eigenenergies and is clearly unphysical. Thus any calculations performed using eq. (4.3.8) must be regarded as inconsistent.

Detailed effects of the approximation 4.3.10 are calculated and discussed in chapters 5, 6 and 7. In the next two sections the consistent approximations $H^{(n)}(R,R')$ and $O^{(n)}(R,R')$ calculated using eq. (4.3.10) are expressed in terms of the quantities $\overline{H}^{(n)}(R,R')$ and $\overline{O}^{(n)}(R,R')$ for the α-α and ^{16}O-^{16}O cases, respectively.

§4.4 Exchange Approximations For α-α Scattering

In the case of identical clusters, $A_1 = A_2 = N$ the wave function (for the GCM kernels) becomes

$$\psi = \frac{N!}{\sqrt{(2N)!}} (A_0+A_1+\ldots+A_N)\mathcal{A}_1\mathcal{A}_2\{\overline{\psi}_1(R/2)\overline{\psi}_2(-R/2)\} \qquad (4.4.1)$$

$$= \frac{N!}{\sqrt{(2N)!}} (A_0+A_1+\ldots+A_N)\psi_1(R/2)\psi_1(-R/2)$$

where $\overline{\psi}_1(R/2)\overline{\psi}_2(-R/2)$ are simple product wave functions centred at $+R/2$ and $-R/2$, respectively. The wave functions $\psi_1(R/2) = \mathcal{A}_1\overline{\psi}_1(R/2)$ and $\psi_2(-R/2) = \mathcal{A}_2\overline{\psi}_2(-R/2)$ are Slater determinants representing the clusters 1 and 2 respectively.

It is easy to see that the total exchange operator, A_N, simply implies changing R to $-R$. Similarly the operators A_{N-1} and A_1 are equivalent with the same parity change so that for N even, the wave function may be written

$$\psi(R) = \frac{N!}{\sqrt{(2N)!}} (1+P_R)(A_0+A_1+\ldots+\frac{A_{N/2}}{2})\psi_1(R/2)\psi_2(-R/2), \qquad (4.4.2)$$

where P_R is the parity operator acting on the generator coordinate R. It is this symmetrisation with respect to R which manifests itself in the exact cancellation of odd parity or odd angular momentum relative motion states. For non-identical particles there is partial cancellation by the same

mechanism which can give rise to a parity dependent effective interaction.

The exchange operators may be defined in terms of the Laplace expansion of determinants (Ayres 1974) in which the (2N x 2N) slater determinant, $\psi(R)$, is expressed as a sum of products of two (N x N) determinants. The first (direct) term is just the product $\psi_1(R/2)\psi_2(-R/2)$. All other terms may be derived from the direct term by performing all possible interchanges of single particle states between the two determinants. Suppose the columns of $\psi_1(R/2)$ are labelled 1 - 4 and the columns of $\psi_2(-R/2)$, 5 - 8 and the permutation operator P_{ij} interchanges the single particle states appearing in columns i and j, then from the Laplace expansion of $\phi(R)$ the exchange operators can be identified as

$$\left.\begin{aligned} A_0 &= 1, \\ A_1 &= \sum_{i=1}^{4}\sum_{j=5}^{8} - P_{ij} \ , \\ \text{and} \quad A_2 &= \sum_{i_1<i_2=1}^{4}\cdots\sum^{4} \sum_{j_1<j_2=5}^{8}\cdots\sum^{8} P_{i_1 j_1} P_{i_2 j_2} . \end{aligned}\right\} \qquad (4.4.3)$$

These exchange operators are all that are required for the α-α problem.

Using these definitions, $H^{(n)}(R,R')$ may be calculated in terms of the known $\bar{H}^{(i)}(R,R')$ by writing

$$(A_0+A_1)^2 = A_0+A_0A_1+A_1A_0+A_1^2. \qquad (4.4.4)$$

Clearly

$$A_0^2 = A_0 \quad , \ A_0A_1 = A_1A_0 = A_1 \qquad (4.4.5)$$

and the remaining problem is

$$A_1^2 = \sum_{i=1}^{4}\sum_{i'=1}^{4}\sum_{j=5}^{8}\sum_{j'=5}^{8} P_{ij}P_{i'j'}. \qquad (4.4.6)$$

To evaluate A_1^2, the summation is divided into three regions:

(i) $i=i'$ *and* $j=j'$, (ii) $i=i'$ *or* $j=j'$ and (iii) $i\neq i'$, $j\neq j'$.

The first region simply gives

$$\{1\} = \sum_{i=1}^{4} \sum_{j=5}^{8} P_{ij}P_{ij} \tag{4.4.7}$$

$$= \sum_{i=1}^{4} \sum_{j=5}^{8} 1 = 16A_0.$$

The second region is more complicated

$$\{2\} = \sum_{i=1}^{4} \sum_{j\neq j'=5}^{8} P_{ij}P_{ij'} + \sum_{i\neq i'=1}^{4} \sum_{j=5}^{8} P_{ij}P_{i'j}. \tag{4.4.8}$$

The product of two permutation operators may be contracted when two of the four indices are identical and using the rule of determinants which states that interchange of any two columns (or rows) simply changes its sign then

$$\left.\begin{aligned} P_{ij}P_{ij'} &= -P_{ij} \\ \text{and} \qquad P_{ij}P_{i'j} &= -P_{ij} \end{aligned}\right\} \tag{4.4.9}$$

so that

$$\{2\} = \sum_{i=1}^{4} \sum_{j\neq j'=5}^{8} -P_{ij} + \sum_{i\neq i'=1}^{4} \sum_{j=5}^{8} -P_{ij} \tag{4.4.10}$$

$$= 6A_1.$$

The third region can be further subdivided into the regions $i<i'$, $i>i'$, $j<j'$ and $j>j'$. This results in four separate sums all of the form

$$\sum_{i<i'=1}^{4} \sum_{j<j'=5}^{8} P_{ij}P_{i'j'}, \tag{4.4.11}$$

where the indices are relabelled accordingly and use has been made of the identity

$$P_{ij}P_{i'j'} = P_{ij'}P_{i'j} \text{ for } i\neq i',\ j\neq j', \tag{4.4.12}$$

so that

$$\{3\} = 4\sum_{i<i'=1}^{4} \sum_{j<j'=5}^{8} P_{ij}P_{i'j'} \tag{4.4.13}$$

$$= 4A_2.$$

Consequently

$$A_1^{\,2} = 16A_0 + 6A_1 + 4A_2. \tag{4.4.14}$$

Using these relationships the n-particle exchange approximations for the GCM kernels, and hence the matrix elements, in the α-α case (N=4) are

$$\left.\begin{aligned} H^{(0)}(R,R') &= \tfrac{1}{35}\,\bar{H}^{(0)}(R,R'), \\ H^{(1)}(R,R') &= \tfrac{1}{35}\{17\bar{H}^{(0)}(R,R')+8\bar{H}^{(1)}(R,R')+8\bar{H}^{(2)}(R,R')\}, \\ H^{(2)}(R,R') &= \bar{H}^{(0)}(R,R')+\bar{H}^{(1)}(R,R')+\bar{H}^{(2)}(R,R') \ \text{(exact)}, \end{aligned}\right\} \tag{4.4.15}$$

where $\bar{H}^{(2)}(R,R')$ is given by $A_2/2$ in eq. (4.4.2).

From equations (4.4.15) it may appear that the *exchange* approximations contribute to the *direct terms* $\bar{H}^{(0)}(R,R')$. This is not so since the direct term defined here is determined by an arbitary choice of one of the thirty-five possible relative coordinates and by allowing exchange other possibilities become asymptotically non-zero. Consequently in any calculation the matching to the external wave function must be normalised appropriately. This is most simply performed by renormalising the exchange contributions $\bar{H}^{(n)}(R,R')$ so that the coefficient of the direct term is always 1 as in the exact, fully antisymmetric, case. The expressions for the overlap kernels are of course analogous with H replaced by O throughout.

§4.5 Exchange Approximations for ^{16}O-^{16}O Scattering

Extending the definition of the exchange operators A_n to allow up to 16 particle exchange one has

$$A_n = \sum_{i_1<i_2<\ldots<i_n=1}^{16} \cdots\cdots \sum_{j_1<j_2<\ldots\, j_n=17}^{16} \sum^{32} \cdots\cdots \sum^{32} (-1)^n P_{i_1 j_1} P_{i_2 j_2} \ldots P_{i_n j_n}. \tag{4.5.1}$$

However for N = 16 only exchange operators up to A_8 need to be considered and it is possible to derive expressions for $H^{(n)}(R,R')$ in terms of the nine known terms $\bar{H}^{(n)}(R,R')$ (n=0,1,...,8).

The integer coefficients involved can be very large so that a procedure has been developed to permit the use of the symbolic algebra code "REDUCE" (Hearn 1972) which has no integer size limitations.

Firstly one notes that all the exchange operators commute and that $A_n A_o = A_o A_n = A_n$. Secondly all products of the form $A_1 A_n$ are calculable by a similar method to that described in §4.4 for A_1^2.

The product summation consists of three regions, the first in which the indices i,j of A_1 both equal one of the summation indices for A_n, i.e. if the summation indices $(i_1, i_2, \ldots i_n)$ and $(j_1, j_2, \ldots j_n)$ are considered to form two sets $\{i_k\}$ and $\{j_k\}$ respectively then in the first region $i \in \{i_k\}$ *and* $j \in \{j_k\}$. In the second region $i \in \{i_k\}$ *or* $j \in \{j_k\}$ and in the third region $i \notin \{i_k\}$ *and* $j \notin \{j_k\}$.

Define $\{I\}$, I = 1,2,3 to be the contribution to the product of the first, second and third regions respectively then

$$\{1\} = \sum_{i=1}^{16} \sum_{j=17}^{32} \sum_{i_1<i_2<..<i_n=1}^{16} \cdots \sum_{j_1<j_2<..<j_n=17}^{32} -(-1)^n P_{ij} P_{i_1 j_1} \ldots P_{i_n j_n}$$

$$\times \left(\sum_{k=1}^{n} \delta_{i i_k} \right) \left(\sum_{k'=1}^{n} \delta_{j j_{k'}} \right) \qquad (4.5.2)$$

$$= \sum_{k,k'=1}^{n} \sum_{i_1<..<i_k<..<i_n=1}^{16} \cdots \sum_{j_1<..<j_{k'}<..<j_n=17}^{32} -(-1)^n \frac{P_{i_1 j_1} \ldots P_{i_n j_n}}{P_{i_k j_{k'}}},$$

where the identities (4.4.9) and (4.4.12) have been used and the division by $P_{i_k j_{k'}}$ indicates that this term is to be omitted from the product. The summations over k and k´ may be performed resulting in the sums over i_k and $j_{k'}$ becoming the sums over all values except $i_1, \ldots, i_{k-1}, i_{k+1} .. i_n$ and $j_1, \ldots, j_{k'-1}, j_{k'+1} .. j_n$, respectively. Thus

$$\{1\} = (16-n+1)^2 A_{n-1} . \qquad (4.5.3)$$

The contribution from the third region is also easily evaluated and is simply the number of ways i,j may be fitted into the sequences $i_1<i_2<\ldots<i_n$ and $j_1<j_2<\ldots<j_n$, such that $i\notin\{i_k\}$ and $j\notin\{j_k\}$, times A_{n+1}. Thus

$$\{3\} = (n+1)^2 A_{n+1}. \tag{4.5.4}$$

For the second region, enumerating the various possibilities is very tedious. However the total number of permutations, $N(A_n)$, involved with each exchange operator is easily calculated:

$$N(A_n) = \binom{16}{n}, \tag{4.5.5}$$

where the bracket is the usual binomial coefficient, and hence the total number of terms in the product A_1A_n is known:

$$N(A_1A_n) = N(A_1)N(A_n). \tag{4.5.6}$$

In the second region only two indices are equal so that there must remain n independent pairs of indices plus one summation which can be performed. Consequently the contribution from the second region must be of the form KA_n where K is an integer. The total number of terms must remain the same therefore

$$K = \frac{N(A_1A_n) - (n+1)^2 N(A_{n+1}) - (16-n+1)^2 N(A_{n-1})}{N(A_n)}. \tag{4.5.7}$$

In this way all products A_1A_n can be determined in terms of A_n, $A_{n\pm1}$ and the coefficients of these expansions are tabulated in appendix C.

Clearly the one-particle exchange approximation is now known:

$$(A_0+A_1)^2 = A_0+2A_1+A_1^2 \tag{4.5.8}$$

The next step is to calculate the two-particle exchange approximation

$$(A_0+A_1+A_2)^2 = (A_0+A_1)^2+2(A_0+A_1)A_2+A_2^2 \tag{4.5.9}$$

The first two terms on the right hand side of eq. (4.5.9) are known and the last is determined by expressing A_2 in terms of A_0, A_1 and A_1^2, from the

expansion of A_1^2, and then using known products:

$$A_2^2 = A_2 \tfrac{1}{4}\{A_1^2 - 30A_1 - 256A_0\} \tag{4.5.10}$$

and then

$$A_2 A_1^2 = (A_2 A_1)A_1 \ , \tag{4.5.11}$$

which is calculated using the already determined products $A_1 A_n$. Having found A_2^2 and hence the two-particle exchange approximation the three-particle approximation is calculated using known products and reducing any new products to those involving A_1. At each stage new products of the form $A_i A_j$ are evaluated in terms of the A_n and may then be used to find the next approximation.

The complete list of exchange approximations calculated by following such a procedure is given in appendix C. The renormalised coefficients E_{ni} for the expansion of $H^{(n)}(R,R')$ in terms of $\bar{H}^{(n)}(R,R')$:

$$H^{(n)}(R,R') = \bar{H}^{(o)}(R,R') + \sum_{i=1}^{8} E_{ni} \bar{H}^{(i)}(R,R') \tag{4.5.12}$$

are given in table 4.1.

From the behaviour of these coefficients it is reasonable to expect that the effects of allowing successively more particles to be exchanged is monotonic and approximately linear contrary to earlier results based on the expansion

$$H^{(n)}(R,R') = \bar{H}^{(o)}(R,R') + \sum_{i=1}^{n} \bar{H}^{(i)}(R,R'), \tag{4.5.13}$$

which has been shown here to be incorrect. The actual phase shifts calculated using eq. (4.5.12) are plotted in chapter 6 and are discussed in chapters 6 and 7. It is believed to be the first time that a dynamical heavy-ion calculation has been performed for correctly interpreted particle exchange approximations.

TABLE 4.1 Particle-exchange approximation coefficients, E_{ni}, for ^{16}O - ^{16}O, normalised such that $E_{oi} = 1$, n = number of exchanged particles.

n	E_{n1}	E_{n2}	E_{n3}	E_{n4}	E_{n5}	E_{n6}	E_{n7}	E_{n8}
1	.12451	.01556	-	-	-	-	-	-
2	.24780	.07396	.01719	.002456	-	-	-	-
3	.36932	.16750	.07071	.02594	.007311	.001219	-	-
4	.48822	.28805	.16755	.09249	.04645	.02008	.006730	.002692
5	.60308	.42667	.30427	.21339	.14424	.09486	.06505	.05509
6	.71157	.57312	.46857	.39247	.33832	.30214	.28135	.27458
7	.80981	.76923	.74894	.73742	.73028	.72591	.72352	.72271
8	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0

CHAPTER 5

α - α ELASTIC SCATTERING

§5.1 Introduction

α-α elastic scattering is often the first test of microscopic methods designed to treat the problem of heavy-ion scattering. This is because the α-particles are tightly bound and can be fairly well represented by the shell model configuration $(1s)^4$ greatly simplifying the calculations, especially if h.o. states are assumed. Similarly, here the α-α scattering problem has been used to develop and test the assumptions used to solve the harder problem of ^{16}O - ^{16}O scattering.

In §5.2 the α-α elastic scattering phase shifts are calculated using the methods described in chapters 2 and 3. No approximations regarding the antisymmetrisation are made other than that described in chapter 2, namely that the asymptotic indistinguishable channels do not overlap because the exchange terms have a finite range, and all matrix elements are calculated within the internal region. These results are tested for stability and convergence with to: (i) the number of basis states μ, (ii) the matching radius a and (iii) the number of terms in the expansion of the coulomb interaction μ_c (see §5.2).

To permit comparison with earlier similar calculations (Baye and Heenen 1974, Canto and Brink 1977) a Volkov force 1 (Volkov 1965) has been used as an effective interaction. This force gives a good fit to the experimental data. Lastly in §5.2, the energy correction for distant levels,

eq. (2.6.10) is tested as a method for reducing the size of matrices required for diagonalisation. In the α-α case, which requires less than five basis states, this is not a problem but it may become very important for larger systems.

In §5.3, the assumption that the exchange contributions may be calculated by integrating over all space (i.e. $a \to \infty$) eq. (3.3.2), is tested directly. It is then shown that these terms are identical to equivalent terms derived from the GCM kernels. In this way, using the results of chapter 4, the 0-, 1-, 2- particle exchange approximations are studied for a Volkov force 1. In §5.3, the "particle-exchange" approximation results using eq. (4.3.8) are also given. In this case the results are very close to the exact calculation for n = 1, *provided not too many basis states are included.* This approximation has no physical interpretation or justification but shows that the longest ranged terms, whatever their origin, are the most important. This statement appears almost self-evident; however exclusion of the shorter-ranged terms (in the matrix elements) can give rise to serious problems such as complex eigenenergies (as occurs in ^{16}O-^{16}O). The approximation is as stated earlier (§4.3) inconsistent.

In §5.4, the effect of forbidden states is studied by using the projection method of §4.2. The α-α scattering phase shifts are calculated using only the direct terms with and without the orthogonality condition, eq. (4.2.4), as an additional constraint. The projected phase shifts are also calculated using the interaction employed by Saito (1969) and are compared with his results.

§5.2 Exact Matrix Elements

The Hamiltonian and overlap matrix elements over the internal region are calculated following the method described in chapter 2. Firstly an arbitrary choice of cluster coordinates is made and integrations are performed over all space for all coordinates except for the relative

separation r, of the centres-of-mass of the two α-particles. The integral over r is confined to a sphere of radius a. The order of integration is: (i) all spin-isospin variables, (ii) all internal coordinates ρ_i, remembering their linear dependence implied by relations (2.2.4) and (iii) integration over the generator coordinates R, R′ and the angular coordinates of r. This leaves a function of r to be integrated from 0 to a which can be treated numerically. In fact even this last integral can be performed analytically for the exchange and $V_D(r)$ contributions if the range of integration is extended to ∞ (see §5.3). Furthermore, since the basis states satisfy natural boundary conditions, the remaining direct contributions to the matrix elements can be evaluated exactly within the internal region by analytical methods.

To demonstrate this procedure, we now detail the calculation of the overlap matrix elements.

The basis state wave function has the form:

$$\Psi_i = \int dR f_i(R)\phi(R) \tag{5.2.1}$$

and the required matrix element is

$$o_{ij} = \langle\Psi_i|\Psi_j\rangle \tag{5.2.2}$$

$$= \iint dR dR' f_i^*(R) f_j(R') \langle\phi(R)|\phi(R')\rangle \ ,$$

where the angular brackets denote integration over the *internal* region. Integrating over spin and isospin with the antisymmetriser on one side only gives

$$\langle\phi(R)|\phi(R')\rangle = \underset{\text{Int. region}}{\iint} dr_1 \ldots dr_8 \left(\frac{2\nu}{\pi}\right)^{12} \exp\{-\nu \sum_{i=1}^{4} (r_i - \frac{R}{2})^2 - \nu \sum_{i=5}^{8} (r_i + \frac{R}{2})^2$$

$$\times 16 \exp\{-\nu \sum_{i=1}^{8} r_i^2 - 2\nu R'^2\} \Big\{ \mathrm{Sinh}(\nu(r_1 - r_5).R') \mathrm{Sinh}(\nu(r_2 - r_6).R')$$

$$\times \mathrm{Sinh}(\nu(r_3 - r_7).R') \mathrm{Sinh}(\nu(r_4 - r_8).R') \Big\} \tag{5.2.3}$$

Inserting cluster coordinates and integrating over the *six* independent ρ_i using

$$\int_{\text{all } r} dr \exp(-\alpha r^2+\beta r.s) = \exp(\frac{\beta^2 s^2}{4\alpha})(\frac{\pi}{\alpha})^{3/2}, \text{ for } \alpha>0 , \tag{5.2.4}$$

gives

$$\langle\phi(R)|\phi(R')\rangle = \int_{r<a} dr \exp\{-4\nu r^2-2\nu(R^2+R'^2)+4\nu r.R\} x 16(\frac{\nu}{\pi})^{3/2}(\text{Jac.})$$

$$x \left\{\cosh(4\nu r.R')-4\cosh(2\nu r.R')\exp(\frac{3\nu R'^2}{4})+3\exp(\nu R'^2)\right\}, \tag{5.2.5}$$

where (Jac.) is the Jacobian factor which can in practice be ignored as it is only a common factor throughout.

The integrals over the generator coordinates in eq. (5.2.2) with $f_i(R)$ defined in §3.2 require the following relations (Abramowitz 1972):

$$\exp(\pm z\cos\theta) = \sum_{n=0}^{\infty} (\pm 1)^n (2n+1)\{(\frac{\pi}{2z})^{\frac{1}{2}} I_{n+\frac{1}{2}}(z)\}P_n(\cos\theta) \tag{5.2.6a}$$

and

$$P_n(\cos\theta_{AB}) = \frac{4\pi}{2n+1} \sum_{m=-n}^{+n} Y^*_{nm}(\Omega_A) Y_{nm}(\Omega_B) , \tag{5.2.6b}$$

where $I_\nu(z)$ is a modified Bessel function and $P_n(z)$ is a Legendre polynomial. Also required is the integral (Magnus *et al* 1966):

$$\int_0^\infty J_\nu(\alpha t)J_\nu(\beta t)\exp(-\gamma t^2)t\,dt = \frac{1}{2\gamma}\exp\left\{-\frac{(\alpha^2+\beta^2)}{4\gamma}\right\} I_\nu(\frac{\alpha\beta}{2\nu}), \text{ Re } \nu > -1 , \text{ Re } \gamma > 0 , \tag{5.2.7}$$

with α and β set to $i\alpha'$ and $i\beta'$ in the Bessel functions $J_\nu(z)$ for integrals involving $I_\nu(\alpha t)$ and $I_\nu(\beta t)$.

The matrix element (omitting the Jacobian factor) becomes:

$$O_{ij} = \tfrac{1}{2}(1+(-1)^L)\exp(\frac{-k_i^2}{8\nu})\{\tfrac{1}{2}\exp(\frac{-k_j^2}{8\nu})\int_0^a j_L(k_i r) j_L(k_j r) r^2 dr$$

$$\frac{-32\sqrt{2}}{5^{3/2}} \exp\left(\frac{-k_j^2}{5\nu}\right) \int_0^a \exp\left(-\frac{6\nu r^2}{5}\right) j_L\left(\frac{4k_j r}{5}\right) j_L(k_i r)\, r^2 dr$$

$$+3\sqrt{2}\exp\left(-\frac{k_j^2}{4\nu}\right)\delta_{L0}\int_0^a \exp(-2\nu r^2) j_0(k_i r)\, r^2 dr\}\delta_{LL'}\delta_{MM'} \,. \qquad (5.2.8)$$

Clearly basis states associated with different asymptotic angular momenta are orthogonal and odd L values give zero matrix elements. This reflects the fact that in the external region the two α-particles look like two identical spinless bosons so that only even parity (even L) relative motion states are permitted. The detailed form of the Hamiltonian matrix element H_{ij} is given in appendix D. It has a form analogous to O_{ij} but is more complicated with parameters depending on the assumed nucleon-nucleon interaction

$$V_{ij}^N = V_o \exp(-\beta(r_i - r_j)^2)(w + bP_\sigma - hP_\tau + mP_M). \qquad (5.2.9)$$

The coulomb interaction can be treated by expanding the 1/r dependence in terms of Gaussian functions:

$$\frac{e^2}{|r_i - r_j|} = \frac{2e^2}{\sqrt{\pi}} \int_o^\infty \exp\,(-\beta^2 (r_i - r_j)^2) d\beta \,, \qquad (5.2.10)$$

which has the radial form of V_{ij}^N. That part of the coulomb interaction which depends on the isospin projection and ensures that only *protons* are involved is correctly treated by setting w = 7/30, m = -2/30 and h = b = 0 in the terms of the matrix element H_{ij} which arise from the interaction V_{ij}^N. The integral over β in eq. (5.2.10) can be performed numerically using Laguerre quadrature which has been found to converge faster for this application than the very similar Hermite integration (Abramowitz 1972). These matrix elements can now be used to solve for the α-α elastic scattering phase shifts using the BD method.

The method was tested for convergence and stability with respect to variation of the number of basis states μ, the matching radius a and the

number of terms μ_c , in the expansion of integral (5.2.10). The convergence of the energy correction procedure (§2.6) was also tested for completeness. In all of these tests a Volkov effective interaction (1 or 6) was used with a Majorana exchange component m = 0.56 and a h.o. parameter $\nu = 0.27033\ fm^{-2}$.

Convergence of the results with respect to the number of basis states is not independent of the channel radius. If the channel radius is large then more basis states are necessary even if the same results can be obtained for a smaller value of a and fewer basis states. To overcome this problem a large number (10) of basis states were chosen and table 5.1 shows the effect on the L = 2 phase shift of allowing the value of a to vary from 5.5 fm to 8.0 fm for various energies spanning the range of interest. Clearly the phases are very stable with respect to the value of a in contrast to the method of Horiuchi (1970) which requires *optimisation of the results*, with respect to the value of a. Thus the value of a can be set at the minimum value at which the phases stabilise so that the number of basis states is minimised although in principle any value of a greater than this will suffice. The minimum permissible value of the matching radius (5.5fm) found here is in agreement with other calculations (Baye and Heenen 1977).

Choosing this minimum value of the matching radius, a = 5.5 fm, convergence with respect to the number of basis states was tested. Table 5.2 shows the effect on the L = 2 phase shift of allowing the value of μ to vary in the range 2 to 10 for several energies. Clearly in the energy region $E_{CM} < 30MeV$, 4 basis states are enough and for $E_{CM} < 15MeV$, 3 are sufficient. Table 5.3 shows the energy eigenvalues (in MeV) for L = 2 and $\mu = 3$. The first column is the straight calculation, while the second and third columns show the effect of including the energy correction to these eigenvalues for the next two basis states using eq. (2.6.10). The last column shows the corresponding energy eigenvalues for $\mu = 5$ and clearly the energy correction is in the right direction and converges rapidly.

The final convergence test was to vary the number, μ_c , of terms in

TABLE 5.1 Stability of the α - α scattering phase shifts with respect to the matching radius a. L = 2, E_{CM} = 3, 15, 30 MeV, 10 basis states and a Volkov force 1. All phases are in radians.

Matching Radius a(fm)	δ_2 E_{CM} = 3MeV	δ_2 15MeV	δ_2 30MeV
5.5	1.932	1.337	0.645
6.0	1.916	1.310	0.622
7.0	1.965	1.350	0.628
8.0	1.985	1.351	0.640

TABLE 5.2 Convergence of the α - α scattering phase shifts with respect to the number of basis states μ. L = 2, E_{CM} = 3, 15, 30 MeV, a = 5.5 fm and a Volkov force 1. All phases are in radians.

No. of Basis States μ	δ_2 E_{CM} = 3MeV	δ_2 15MeV	δ_2 30MeV
2	1.809	1.147	0.500
3	1.920	1.285	0.545
4	1.928	1.304	0.602
5	1.930	1.318	0.636
7	1.931	1.330	0.640
10	1.932	1.337	0.645

TABLE 5.3 Test of the energy correction method for the eigenvalues as extra states ϕ_4 and ϕ_5 are approximately included. Column 1 for just 3 basis states, columns 2 and 3 the new eigenvalues as ϕ_4 and ϕ_5 are added and column 4 the solution for 5 basis states. All energies are in MeV.

Eigenvalue	E_i $\mu = 3$	E_i $+ \phi_4$	E_i $+ \phi_4 + \phi_5$	E_i $\mu = 5$
E_1	2.98	2.76	2.75	2.67
E_2	19.47	19.32	19.31	19.20
E_3	46.00	44.30	44.30	44.40

TABLE 5.4 Convergence of the α - α scattering phase shifts with respect to the number of terms in the expansions of the coulomb interaction μ_C. L = 2, E_{CM} = 3,15, 30 MeV, a = 5.5 fm and a Volkov force 6. All phases are in radians.

No. of terms μ_C	δ_2 E_{CM} = 3MeV	δ_2 15MeV	δ_2 30MeV
0	2.75	1.68	.92
2	2.69	1.59	.82
4	2.52	1.46	.74
6	2.38	1.40	.71
8	2.37	1.39	.70
10	2.39	1.40	.70

the expansion of eq. (5.2.10) using Laguerre integration (Abramowitz 1972). Table 5.4 shows how the phase shift for L = 0 changes as the value of μ_c is varied from 0 to 10 for several energies. It is seen that $\mu_c = 6$ is sufficient and the full phase shifts may now be calculated.

Using the minimum values of a, μ and μ_c consistent with convergence, the elastic scattering phase shifts for L = 0, 2, 4, 6 and the Volkov force 1 were calculated and are the solid lines plotted in figures 5.1 and 5.2. Also plotted are phase shifts taken from Baye and Heenen (1974 b), dot-dashed curves, phase shifts taken from Canto and Brink (1977), dashed lines and points with error bars, obtained from a phase shift analysis of experimental data, from the review of Afzal *et al* (1969).

The calculated results are all in good agreement amongst themselves and with experiment. The reason for the small discrepancies between the calculated results is not known but may be due to small differences in certain parameters or fundamental constants and also errors due to extracting data from published diagrams.

In this section it has been shown that the BD method may be employed in conjunction with the GCM wave functions to give accurate converged phase shifts in agreement with other microscopic calculations. Only a small number of basis states are required (thus saving computer time and space) especially if the energy correction (§2.6) is employed. A more detailed discussion of all these points is made in chapter 7.

§5.3 Particle Exchange Approximations

Provided the matching radius is large enough (in this case $\geq$ 5.5 fm), the upper limits of the second two integrals in eq. (5.2.8) which arise from exchange terms may be extended to ∞ without any loss of accuracy. This is due to the presence of the $\exp(-\alpha r^2)$ term in each integrand and this approximation was tested directly by comparing the value of the numerical integral over the finite range with the analytical value which can be

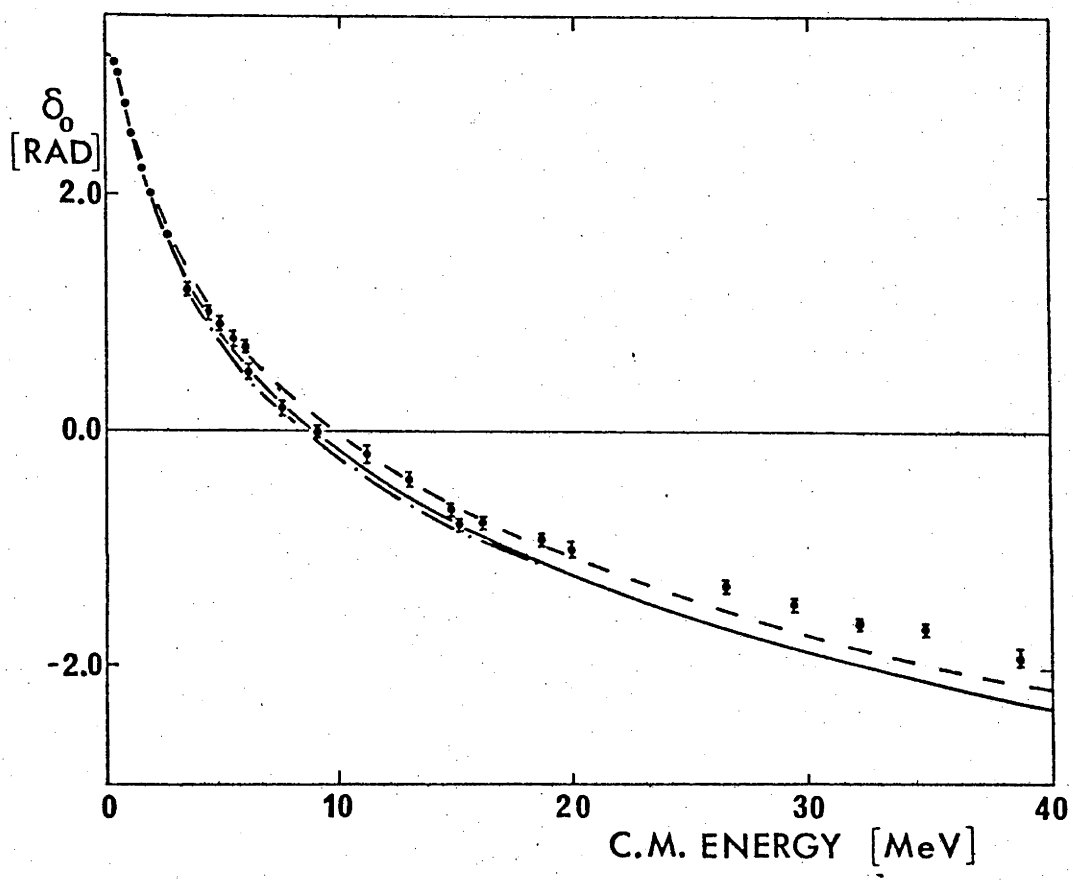

FIGURE 5.1 L = 0 phase shift for α - α elastic scattering. Solid curve is present results, dashed curve results taken from Canto and Brink (1977) and the dot-dashed curve is MRM calculated phases of Baye and Heenen (1974). Points denote phase shift analyses (Afzal *et al* 1969).

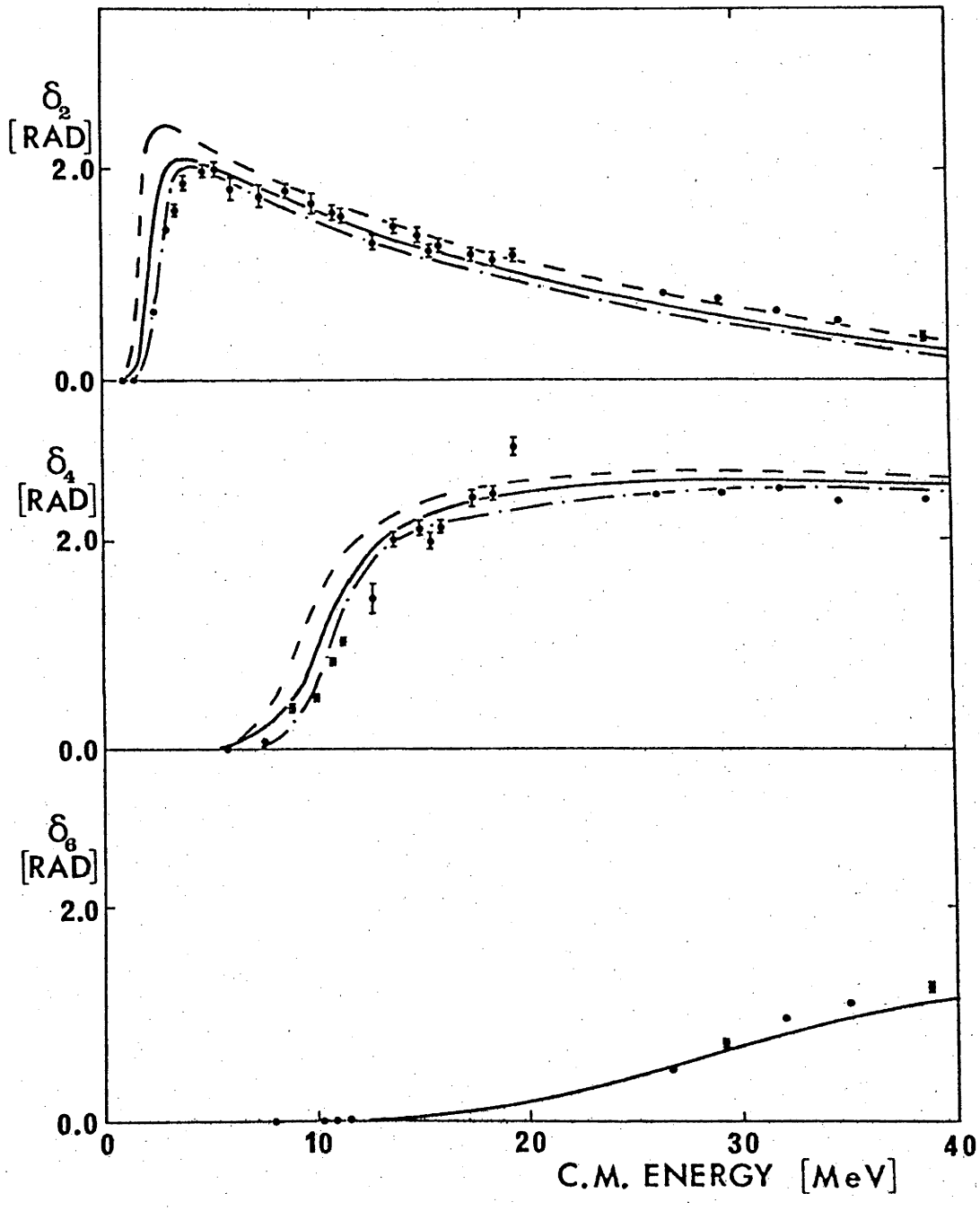

FIGURE 5.2 L = 2, 4 and 6 phase shifts for α - α elastic scattering. Same notation as in fig. 5.1.

obtained (see below) for $a \to \infty$. It was found that in all cases the difference between the two values was less than one part in 10^5 with no discernable change in the calculated phase shifts.

By extending the range to infinity these integrals can easily be performed analytically using eq. (5.2.7). As mentioned earlier, the direct term may also be evaluated analytically because the wave numbers k_i are such that n.b.c.'s are satisfied:

$$b_c j_L(k_i a) - k_i a\, j_L'(k_i a) = 0 \ , \tag{5.3.1}$$

where $b_c = b - 1$. This allows eq. (11.4.5) of Abramowitz (1972) to be used giving

$$\int_o^a j_L(k_i r) j_L(k_j r) r^2 dr = \frac{a}{2k_i^2}\{(b_c+\tfrac{1}{2})^2 + k_i^2 a^2 - (L+\tfrac{1}{2})^2\} j_L(k_i a)\delta_{ij} \tag{5.3.2}$$

so that the direct terms of the basis wave functions are orthogonal over the internal region. In the same way all the Hamiltonian terms can be evaluated using eq. (5.2.7) or (5.3.2) which makes the calculation of the matrix elements very fast and accurate thus saving considerably computer time.

Since the exchange terms may be calculated over all space they may also be determined from the GCM kernels. To show this, we write explicitly the GCM overlap kernels for the α-α case.

These kernels are reported in the literature (e.g. Lumbroso 1974) but are repeated here so that their general structure may be discussed. The overlap GCM kernel is

$$O(R,R') = \exp(-\nu(R^2+R'^2))\ 2\{\mathrm{Cosh}\ (2\nu R.R') - 4\mathrm{Cosh}(\nu R.R') + 3\} \tag{5.3.3}$$

and the Hamiltonian kernel is detailed in appendix E. Integrating over r in eq. (5.2.5) for $a \to \infty$ using eq. (5.2.4) gives

$$\lim_{a \to \infty} \langle \phi(R) | \phi(R') \rangle = O(R,R') \tag{5.3.4}$$

as it must by definition. The exchange terms of eq. (5.2.8) can be identified

with the exchange terms of eq. (5.3.3) (i.e. those with finite range) and henceforth the GCM kernels may be used to determine the exchange contributions.

Each term of the kernel $O(R,R')$ has an exponetial factor of the form

$$\exp\{\pm(2-n)\ \nu R.R'\}\ , \qquad (5.3.5)$$

where n = 0, 1, 2. These are the terms due to A_0 , A_1 , A_2 acting on only one side of the matrix elements and are the $\bar{O}^{(0)}(R,R')$, $\bar{O}^{(1)}(R,R')$ and $\bar{O}^{(2)}(R,R')$ contributions, respectively. Similarly, by letting $\beta \to o$, all the Hamiltonian terms can be identified and the particle exchange approximations derived in §4.4 may be applied.

Figures 5.3 and 5.4 show the n-particle exchange approximate phase shifts for L = 0, 2, 4, 6 using the Volkov force 1 and including the coulomb term. The solid curves are the exact, or fully antisymmetric, n = 2 results, the dashed curves are the direct only or n = 0 phase shifts and the dot-dashed lines are the phase shifts when up to one-particle (and one-hole) exchange is permitted.

In the L = 0 and 2 cases, the exchange contributions are clearly very important and all act in the same direction. In this case the phase shifts *increase* as exchange is included, which corresponds to an extra *attraction* in the effective interaction. Contrary to these results LeMere *et al* (1979) find an alternating effect as more particles are exchanged in the similar system ^{3}He - α. However, this effect is probably spurious arising from the misidentification of the exchange contributions as discussed earlier.

For L = 4 and 6, the n = 0 phases are very close to the exact result and the exchange contributions have only a small but equally important effect. Below a certain energy, the exchange terms act repulsively although the effect is too small to be plotted for L = 6.

Figure 5.5 shows the L = 0 phase shifts calculated using the incorrect particle-exchange approximations eq. (4.3.8). The dot-dashed line corresponds to n = 0, the dashed to n = 1 and the solid line to n = 2. This implies

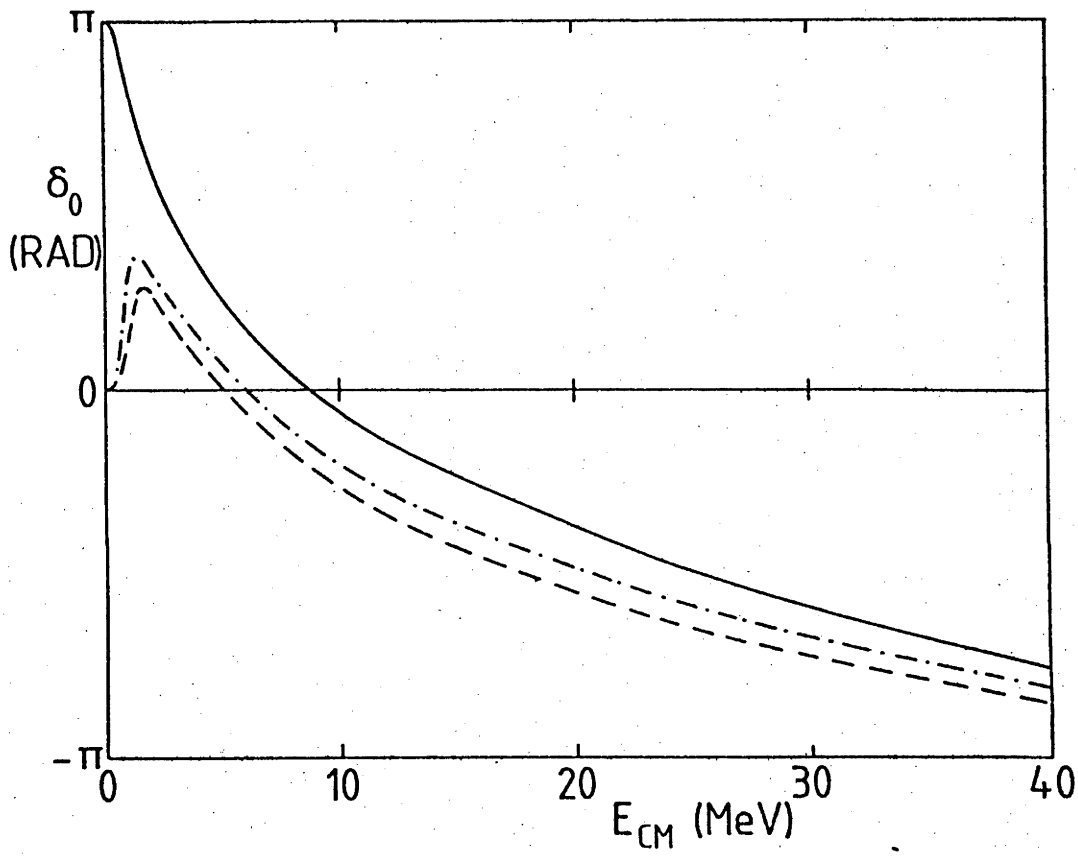

FIGURE 5.3 L = 0 phase shift for α - α scattering for different n-particle exchange approximations. Solid curve is the result of a fully antisymmetric (n = 2) calculation. Dashed curve is the result for the no-particle exchange (n = 0) approximation and the dot-dashed curve for the 1-particle exchange approximation.

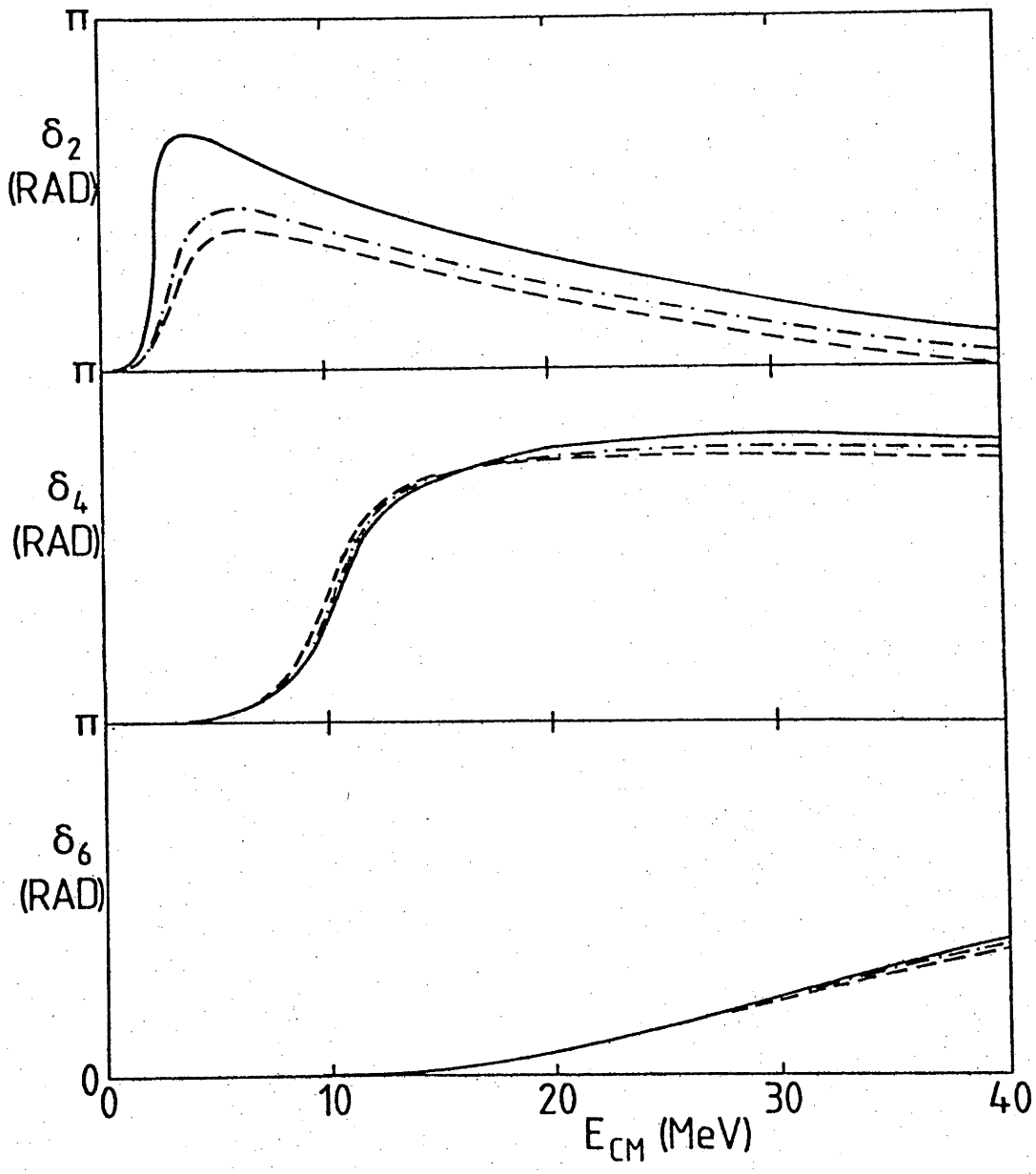

FIGURE 5.4 L = 2, 4 and 6 phase shifts for α - α scattering for different n-particle exchange approximations. Same notation as in fig. 5.3.

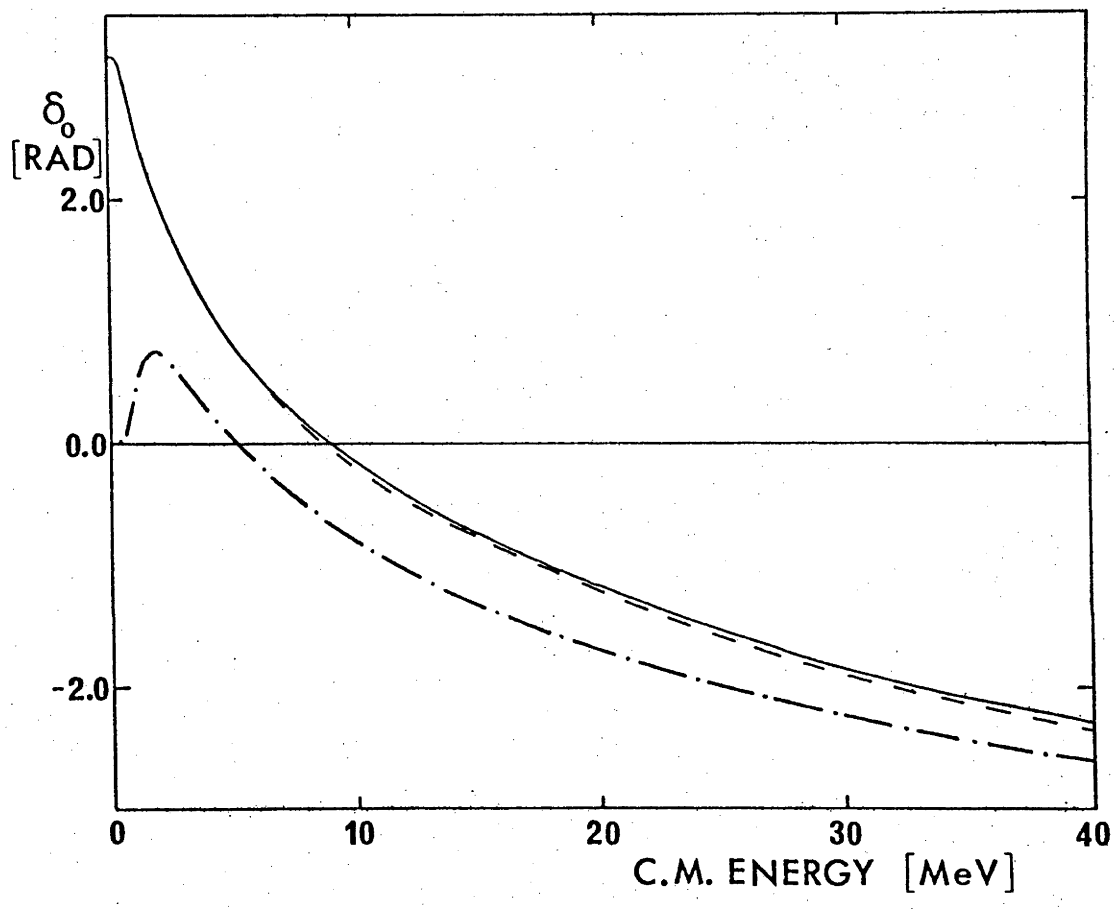

FIGURE 5.5 L = 0 phase shift for α - α scattering for different n-particle exchange approximations using the inconsistent identification of terms eq. (4.3.8). Solid curve is n = 2, dashed curve n = 1 and dot-dashed curve n = 0.

that the contributions from the shortest ranged terms $\bar{H}^{(2)}(R,R')$ and $\bar{O}^{(2)}(R,R')$ are very small in this particular case. However, this is not always true since the equivalent calculation for ^{16}O - ^{16}O scattering cannot be made for $n < 6$ ($L = 12$) without giving rise to complex energies. All these results are discussed further in chapter 7.

§5.4 Projection of Forbidden States

In the α-α system, there are forbidden states of relative motion for only two values of the angular momenta, i.e. $L = 0$ and 2. These are also the only values for which the 0-particle exchange phase shifts are a poor approximation to the exact results and for $L \geq 4$ the direct potential $V_D(r)$ must be close to the exact effective interaction. This is the basis of the original orthogonality condition model, namely that the major effect of the particle exchange is to force the wave function to be orthogonal to the forbidden states.

In the α-α case this hypothesis was tested directly. Using the BD method, solving the elastic scattering problem for the direct potential $V_D(r)$ ($n = 0$ approximation) automatically finds all bound states which the potential may support. In this case for $L = 0$ there are bound states at about -11 and -42MeV and for $L = 2$ one bound state near -14MeV.

Using the projection method described in §4.2 to ensure that the eigensolutions satisfy the orthogonality condition (OC) it is found that these bound states "disappear" and a corresponding number of very large magnitude eigenvalues are found. This indicates that the bound states are close in form to the forbidden states (for $r < a$) and are therefore projected out of the energy range of interest. The large magnitude eigenvalues correspond to the redundant states which can appear at any energy but do not affect the phase shifts (Buck *et al* 1977). Since these bound states are orthogonal to all other eigenstates, the positive energy eigenstates must be nearly orthogonal to the forbidden states so that the OC has

little effect in the positive energy region. This is precisely the result indicated in figures 5.6 and 5.7 and as found by Buck *et al* (1977).

The solid curve in figure 5.6 is the L = 0 phase shift calculated with the OC imposed and the interaction used by Saito (1969). The dot-dashed curve are the corresponding results of Saito which are in good agreement especially at low energies. The dashed line represents the calculation using only the direct potential without the OC and shows that the effect of removing the forbidden states is small.

Figure 5.7 exhibits the L = 0 and 2 phases for similar calculations using the Volkov force. The solid lines are the exact results and the dashed lines correspond to the n = 0 results. The dot-dashed curves are the phases for the direct potential plus the constraint of the OC and clearly it is seen that projecting out these states is not very important. In each case the change in the phase due to the OC is positive which is a general result proved by Englefield and Shoukry (1974). They also discuss the possible removal of a bound state and find a generalisation of Levinson's theorem which states that in calculating the zero energy phase shift, the forbidden states must be included as well as any bound states, so that in this case $\delta_0(E_{CM} = 0) = 2\pi$ and $\delta_2(E_{CM} = 0) = \pi$.

More recent calculations using the OCM (e.g. Tanabe *et al* 1975) give improved results because an effective potential has been used and not *only* the direct potential plus the orthogonality condition.

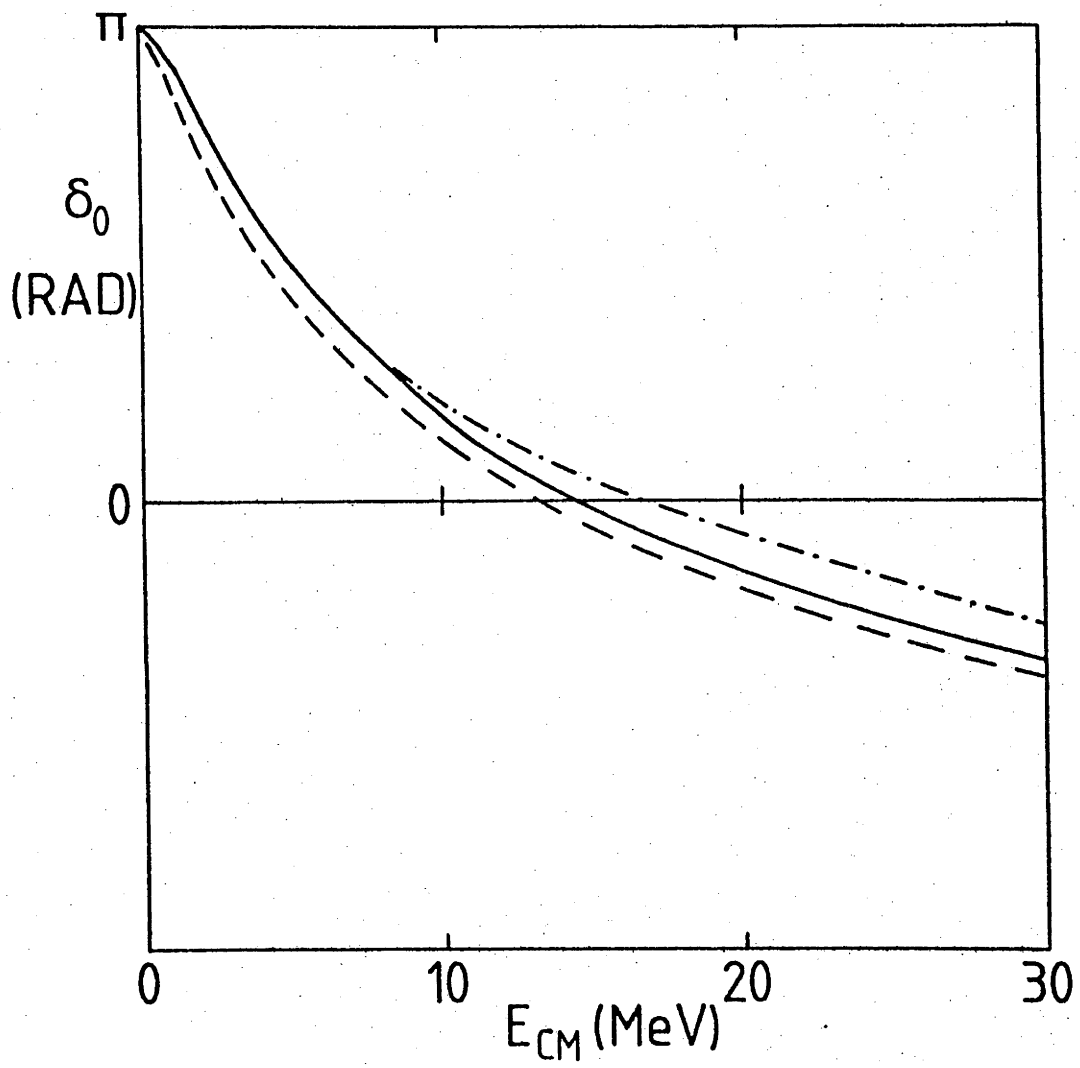

FIGURE 5.6 L = 0 phase shift for α - α scattering using the effective interaction of Saito (1969) and the OC. Solid curve is present results with the OC. Dot-dashed curve equivalent results from Saito (1969) and the dashed curve present results without the OC.

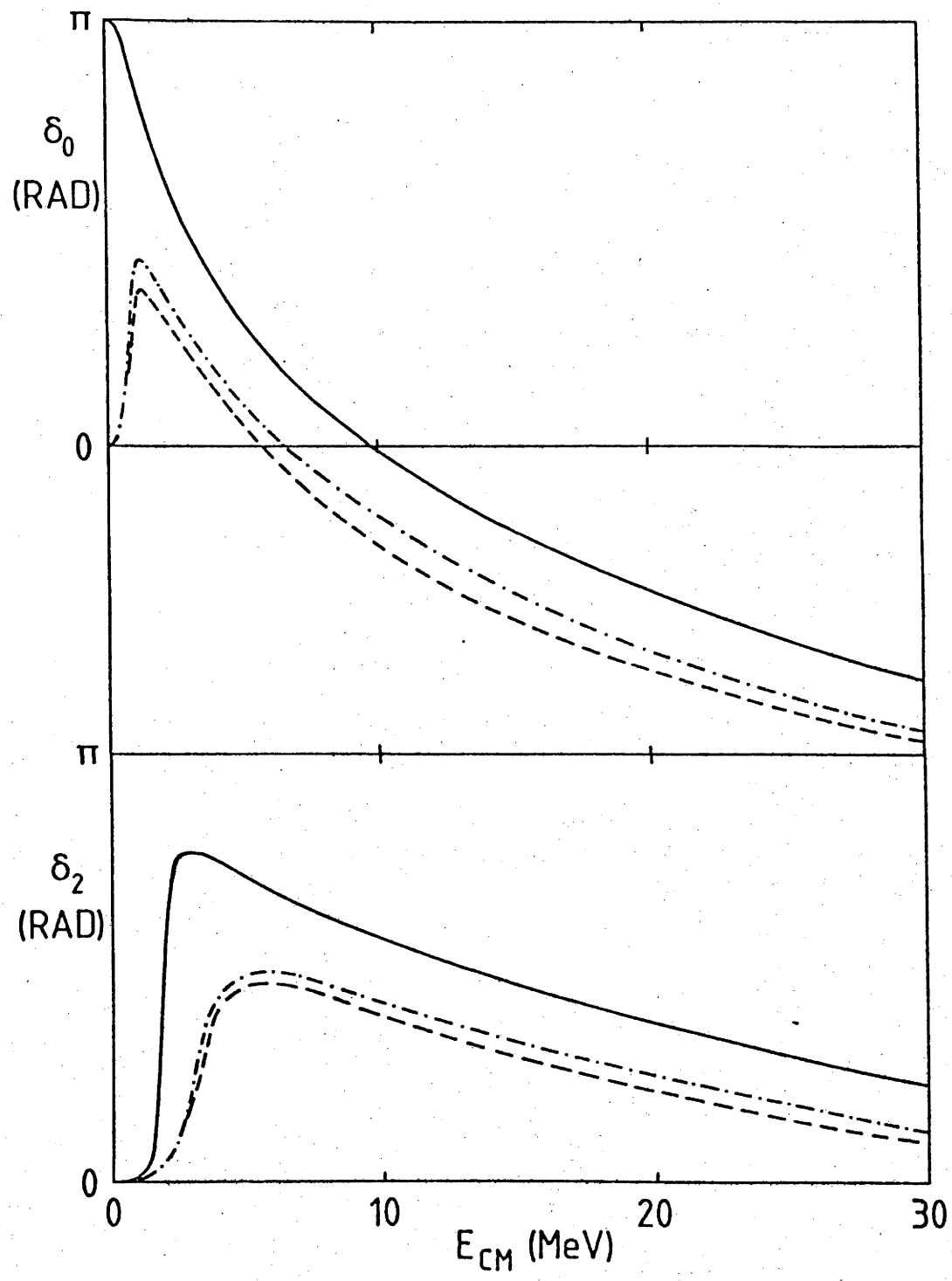

FIGURE 5.7 L = 0 and 2 phase shifts for α - α scattering with a Volkov force. Solid curve is the result of an exactly antisymmetric calculation. Dashed curve is using the direct potential only (n = 0) and the dot-dashed curve for the direct potential plus the OC.

CHAPTER 6

^{16}O - ^{16}O ELASTIC SCATTERING

§6.1 Introduction

The ^{16}O - ^{16}O and α - α systems are very similar if simple closed shell nuclei are assumed so that the total wave function may be described by a single Slater determinant. However the oxygen nuclei involve many more particles and 1p h.o. orbitals thus making the evaluation of the matrix elements when expressed in terms of cluster coordinates extremely difficult. To overcome this particular problem, the result of chapter 5, that the exchange terms may be derived from the GCM kernels, is used. This approach clearly becomes exact as the channel radius $a \to \infty$.

Many similar calculations have been performed using various techniques related to either the RGM (Friedrich 1974a, Ando *et al* 1979) or the GCM (Tohsaki *et al* 1975, Baye and Heenen 1977b, Canto 1977). The introduction of a phenomenological imaginary potential (Baye and Heenen 1977) or a smooth cut-off model (Ando *et al* 1979), to approximate for absorption, permits such microscopic methods to give a qualitative description of the experimental data.

In this chapter the ^{16}O - ^{16}O elastic scattering phase shifts are calculated for the fully antisymmetric wave function and are then analysed in terms of the number of nucleons exchanged in order to determine the most important terms and effects which must be included in any approximate method. Since the emphasis here will be on the structure of the various

terms rather than describing experimental data, the coulomb interaction has been ignored in most of the calculations to save considerable computing time. This clearly affects the actual values of the phase shifts but should not change the importance or otherwise of the various exchange terms. To establish the method, the results of this calculation are compared with Friedrich (1974a) where only the direct coulomb interaction is included. In a detailed comparison of various effective nucleon-nucleon interactions *for this application,* Ando *et al* (1979) conclude that a Volkov force 2 with Majorana exchange component m = 0.65 should give the most consistent results and this choice has been made for most of the earlier investigations. Another interaction commonly used in this type of calculation is the Brink and Boeker force B_1. Both these interactions have been fitted to light ion data, e.g. the binding energy of ^{4}He; however the B_1 potential has also been adjusted to give the correct binding energy per nucleon in nuclear matter. Therefore this force may give a better account of compression effects during large overlap of the nuclei. In this chapter calculations are performed using both effective interactions (see appendix B for parameters) since, although the folded potentials arising from each interaction (see figure 3.1) are very different, the fully antisymmetric results are similar. This has been pointed out before (Weiguny 1977) and is discussed further in chapter 7.

§6.2 ^{16}O - ^{16}O Matrix Elements and Results

Using the methods described in chapter 3, the GCM kernels for the ^{16}O - ^{16}O scattering have been calculated and the matrix B, its inverse B^{-1} and the necessary one- and two-body matrix elements are given in appendix F. The resultant kernels have far too many terms ($\sim 10^4$) to tabulate here. In the computer, the kernels were stored as integer coefficients of terms of the general form:

$$Z(R,R') = d \exp\{-\nu(aR^2 + bR'^2)\}\,(\nu R.R')^i (\nu R^2)^j (\nu R'^2)^k$$

$$\times \begin{cases} \mathrm{Cosh}(c\nu R.R') & i \text{ even} \\ \mathrm{Sinh}(c\nu R.R') & i \text{ odd} \end{cases} \qquad (6.2.1)$$

where i, j, k are integers and a, b, c, d are real coefficients which depend on the parameters of the two body force in the case of the potential terms.

For the overlap kernel $O(R,R')$ the coefficients c are given by

$$c = \frac{(8-n)^2}{64}\ , \qquad (6.2.2)$$

where n = 0, 1, ..., 8 and correspond to taking A_0 , A_1 , ..., A_8 respectively on one side only of the matrix element. Thus the terms may be separated into the 9 groups $\bar{O}^{(n)}(R,R')$ defined in chapter 4, and the particle exchange approximations may be expanded in terms of these groups. Similarly, the full Hamiltonian GCM kernel may be separated by letting $\beta \to 0$ as in the $\alpha - \alpha$ problem and noting that all the coefficients c have the general form (6.2.2).

Having evaluated the GCM kernels and identified all the exchange terms, the matrices *H* and *O* may be calculated by substituting $H(R,R')$ and $O(R,R')$ respectively into eq. (3.2.2) and integrating over the generator coordinates R and R'. The direct terms may be calculated in an analogous way to that employed for the $\alpha - \alpha$ problem:

$$O^D_{ij} = \left(\frac{\pi}{\nu}\right)^{3/2} \frac{1}{4} \exp\left\{\frac{-(k_i^2+k_j^2)}{32\nu}\right\} \int_o^a j_L(k_i r)\, j_L(k_j r)\, r^2 dr \qquad (6.2.3$$

$$= \left(\frac{\pi}{\nu}\right)^{3/2} \exp\left(\frac{-k_i}{16\nu}\right) \frac{a}{8k_i^2} \{(b_c+\tfrac{1}{2})^2 + k_i^2 a^2 - (1+\tfrac{1}{2})^2\} j_L^2(k_i a)\,\delta_{ij}\ ,$$

$$H^D_{ij} = \left\{\frac{\hbar^2 k_i^2}{16m} + 2(\text{B.E.}^{16}\text{O})\right\} O^D_{ij} + (\text{terms from } V_D(r)), \qquad (6.2.4)$$

where the superscript D means that these are matrix elements corresponding

to the direct terms only. The $V_D(r)$ terms are those arising from the two-body potential acting between particles located in different clusters. These give rise to the potential $V_D(r)$ as defined in chapter 3 which may be used to calculate this contribution. Alternatively, because the effective interaction is finite-ranged, the GCM kernels may be used and this is the method employed here.

To calculate the $V_D(r)$ term and the exchange contributions to the matrix elements the first integral in eq. (3.3.2) is required for the general term $Z(R,R')$:

$$I_{mn} = \int dR dR' j_L(k_m R) Y^*_{LM}(\Omega_R) j_L(k_n R') Y_{LM}(\Omega_{R'}) Z(R,R'). \qquad (6.2.5)$$

The expression for $Z(R,R')$ may be rewritten in the form:

$$Z(R,R') = d\left(\frac{\partial}{\partial c}\right)^i \left(-\frac{\partial}{\partial a}\right)^j \left(-\frac{\partial}{\partial b}\right)^k \exp\{-\nu(aR^2 + bR'^2)\}\, \mathrm{Cosh}(c\nu R.R') \qquad (6.2.6)$$

where i, j and k are the exponents of $(\nu R.R')$, (νR^2) and $(\nu R'^2)$, respectively. The integral I_{mn} is then given by

$$I_{mn} = d\left(\frac{\partial}{\partial c}\right)^i \left(-\frac{\partial}{\partial a}\right)^j \left(-\frac{\partial}{\partial b}\right)^k I_o\,, \qquad (6.2.7)$$

where I_o is the integral of eq. (6.2.5) with $Z(R,R')$ such that $i = j = k = 0$ and $d = 1$. The integral I_o can be evaluated analytically:

$$I_o = \frac{2\pi^2}{\nu^2(4ab-c^2)} \left(\frac{\pi}{2c\nu k_m k_n}\right)^{\frac{1}{2}} \exp\left\{\frac{-(bk_m^2+ak_n^2)}{\nu(4ab-c^2)}\right\} I_{L+\frac{1}{2}}\left(\frac{c\, k_m k_n}{\nu(4ab-c^2)}\right), \qquad (6.2.8)$$

where $I_{L+\frac{1}{2}}(Z)$ is a modified Bessel function. Making the substitutions:

$$x = \frac{k_m^2}{16\nu}\,,\quad y = \frac{k_n^2}{16\nu} \text{ and } h = \frac{c^2}{64} \qquad (6.2.9)$$

and using from Buchholz (1969) the relationship:

$$\sum_{\lambda=0}^{\infty} \frac{\lambda!}{\Gamma(1+\mu+\lambda)} h^{\lambda} L_{\lambda}^{(\mu)}(x) L_{\lambda}^{(\mu)}(y) = (1-h)^{-1} (xyh)^{-\frac{1}{2}\mu} \exp\{-\frac{h(x+y)}{1-h}\} x\, I_{\mu}(\frac{2(xyh)^{\frac{1}{2}}}{1-h}),$$

(6.2.10)

where $L_{\lambda}^{(\mu)}(x)$ is a generalised Laguerre polynomial and $\Gamma(\alpha)$ is the usual gamma function, gives:

$$I_o = \frac{\pi^{5/2}}{512\nu^3} (xy)^{L/2} \exp\{-4(\frac{x}{a} + \frac{y}{b})\}$$

$$x \sum_{\lambda=0}^{\infty} \frac{\lambda!}{\Gamma(\lambda+L+3/2)} h^{\lambda+L/2} (\frac{16}{ab})^{\lambda+L+3/2} L_{\lambda}^{(L+\frac{1}{2})}(\frac{4x}{a}) L_{\lambda}^{(L+\frac{1}{2})}(\frac{4y}{b}) \qquad (6.2.11)$$

With I_o expressed in this form, it is a relatively simple matter, using the recurrence relations for Laguerre polynomials, to express the general integral I_{mn} of eq. (6.2.5) as a series of Laguerre polynomials. For most values of the parameters a, b and c involved, the series may be truncated at $\lambda \leq 50$ although for the direct potential terms, summation to higher values of λ may be necessary.

To find the minimum number of basis states required for each L-value, the above method was used to calculate phase shifts for scattering from the folded potential $V_F(r)$ derived from the Volkov force 2 and the results were compared with the corresponding phases obtained by integrating the Schrödinger equation from r = 0 to a as in usual optical model calculations. No additional basis states are required when exchange terms are included since, for this effective interaction, the Pauli exchange acts repulsively thereby reducing the depth of the interaction and thus reducing the "perturbation" to be diagonalised in terms of the plane wave states. This comparison also serves as a test of the accuracy of the method and it has been found to reproduce the optical model (using $V_F(r)$) phases to any desired accuracy but at the cost of large numbers of basis states. For L = 4, 12 and 20, the required number of basis states was found to be 35, 30 and 25,

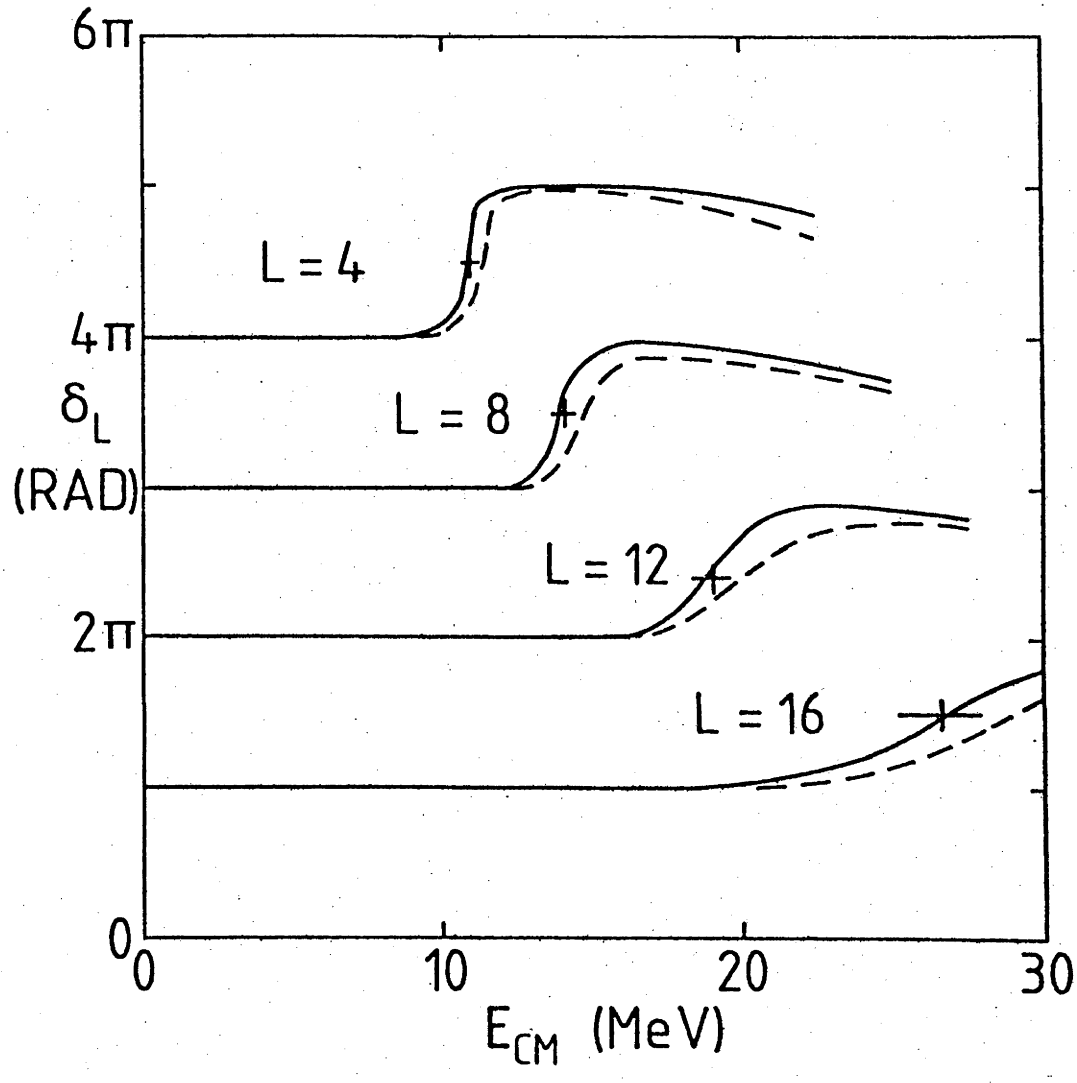

FIGURE 6.1 L = 4, 8, 12 and 16 phase shifts for ^{16}O - ^{16}O elastic scattering using a Volkov force. Solid curves are present results, dashed curve those of Friedrich (1974a) and the crosses represent positions and widths of resonances from Friedrich (1975).

respectively, This decreasing number of basis states required arises from the increasing centrifugal barrier for larger L-values.

To test the correctness of the method for composite particle scattering calculations, the fully antisymmetric ^{16}O - ^{16}O elastic scattering phase shifts have been calculated and compared with the results of an earlier calculation (Friedrich 1974a). For this comparison the coulomb interaction was included in the direct terms but not in the exchange terms and a Volkov force 2 with m = 0.65 and ν = .20029 was used which is very close to that used by Friedrich. In figure 6.1 the solid lines are the results of the present work and the dashed lines are phases taken from Friedrich. In an erratum to this paper (Friedrich 1975) it is reported that the earlier published phase shifts were slightly in error. The positions and widths of the corrected resonances are represented by the crosses and clearly the corrected phases would be in very close agreement with the present work. Moreover, in a calculation including the coulomb interaction in all terms, Canto (1977) compares his results with phase shifts from Friedrich (1974b) and finds good agreement. In this way, it can be seen that the results reported here are not only in close agreement with a nearly equivalent study but also with other more complete calculations. These results are discussed further in chapter 7.

The E_{CM} = 0 values of the phase shifts drawn in figure 6.1 are arbitrary, chosen entirely for convenience so that the phases are equally spaced. The true zero energy phase shifts may be calculated using a generalised Levinson's theorem (Swan 1955, Englefield and Shoukry 1974) which states that:

$$\delta_L(E_{CM} = 0) = (n + m)\pi \ , \qquad (6.2.12)$$

where n is the number of bound states and m is the number of forbidden states. In the solution of the scattering problem by diagonalising the Hamiltonian matrix, for a sufficiently complete basis, any bound states are automatically determined and are easily counted. Table 6.1 gives all the

TABLE 6.1 $E_{CM} = 0$ phases for $^{16}O - ^{16}O$ scattering calculated using the modified Levinson's theorem for all figures appearing in chapters 6 and 7. The V_2 refers to values for the Volkov interaction, B_1 those for the Brink and Boeker interaction and the last row are values for no force.

Interaction and Figure number	δ_4	δ_8	δ_{12}	δ_{16}	δ_{20}
V_2, 6.1	10π	8π	6π	4π	2π
V_2, 6.2 - 6.5	13π	-	8π	-	3π
V_2, 7.3	11π	-	7π*	-	π
B_1, 6.2 - 6.5	10π	8π	6π	4π	2π
B_1, 7.3	10π	8π	6π	4π	2π
0, 7.2	10π		6π		2π

* $\delta_{12}(E_{CM} = 0) = 6\pi$ for the folded potential $V_F(r)$.

E_{CM} = 0 phase for the different L values and the various forces appearing throughout chapters 6 and 7.

§6.3 Particle Exchange Approximations

Using the results of §4.5 the phase shifts for different particle exchange approximations have been calculated. For this investigation the coulomb interaction was ignored entirely thereby saving considerable computer time. Although leaving out these terms shifts the resonances and phases to lower energies, any general effects of the Pauli exchange will still be present. Partially including the coulomb interaction, as in §6.2, is inconsistent and may introduce spurious effects.

The effects of the exchange terms have been studied for various systems (Ando *et al* 1975, LeMere *et al* 1977, LeMere and Tang 1979). In all this work an inconsistent identification of the n-particle exchange approximation was made and an alternating effect on the phase shifts with increasing values of n was found. This result is entirely spurious and arises from using inconsistent approximations as described in chapter 4.

Using the properly consistent approach of eq. (4.3.10), the L = 4, 12 and 20 phase shifts have been calculated in all the n-particle exchange approximations, n = 0, 1, ..., 8.

Figure 6.2 shows the phases for several L-values obtained for both the Volkov 2 and B_1 interactions. The solid lines are the results using fully antisymmetric wave functions (n = 8) and the dashed lines correspond to the phase shifts using only the direct terms (n = 0).

It is seen that the exchange terms can change both the positions and widths of the resonances significantly thus leading to corresponding large effects on the excitation functions in that region. From a physical viewpoint, the change in width may mean the difference between the resonance being observable or not; if the resonance is too narrow or too broad it will not be observed above the background. If the shift in the position of

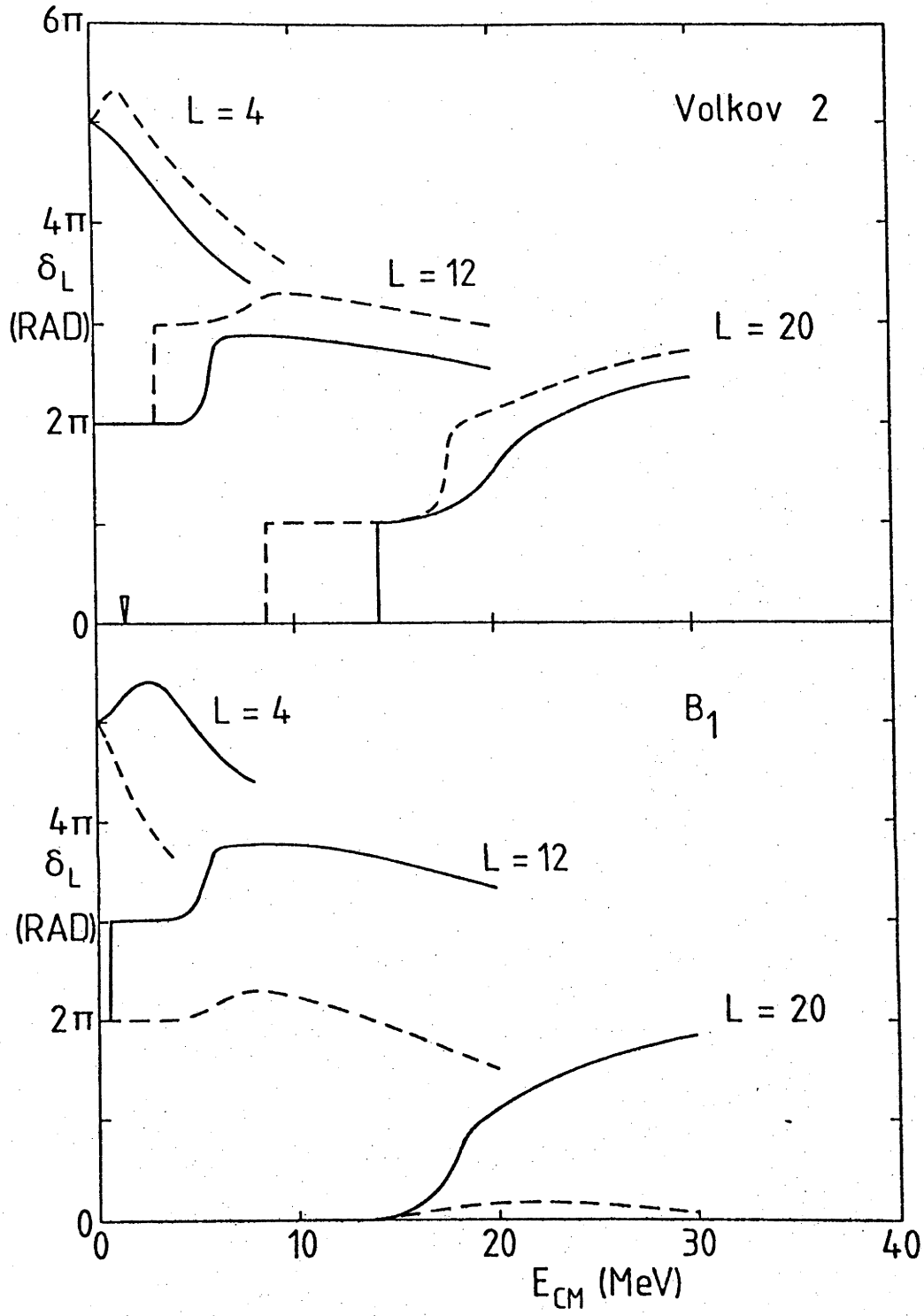

FIGURE 6.2 L = 4, 8 and 12 phase shifts for ^{16}O - ^{16}O scattering using two effective interactions and allowing no-exchange (n = 0) or full exchange (n = 8). Solid curves are the n = 8 results and the dashed curve the n = 0 results. The arrow denotes an extra resonance for the L = 20, n = 8 phase shift. The upper phases are using a Volkov force 2 and the lower using the Brink and Boeker force B_1.

a resonance is sufficient to bring an otherwise bound state into the positive energy region (e.g. L = 20) then antisymmetrisation will give rise to an additional resonance.

Another important result is that the exchange contributions may have opposite effects for different two-body interactions. For the Volkov potential 2 the phases are decreased showing that the exchange terms contribute *repulsively* whereas for the Brink and Boeker potential B_1 the exchange terms contribute *attractively*. This difference has been noted before (Schultheis and Schultheis 1978) and consequently one cannot assume that the effects of polarisation of the single particle states are partly or wholly cancelled by particle exchange (Fleckner and Mosel 1977).

In the case of the B_1 force the exchange terms create a resonance not by transferring a bound state to the positive energy region but by making the effective interaction more attractive so that is is able to support a quasi-bound state (Baye and Heenen 1977).

Clearly for both effective nucleon-nucleon potentials the inclusion of full antisymmetrisation is important. Antisymmetrisation may introduce (or remove) resonances into (from) the scattering region by various mechanisms depending on the two-body interaction. Finally, the exchange terms become less important for sufficiently high L-values since they correspond to large impact parameters so that the overlap of the heavy-ions and the effect of Pauli principle are small.

Figures 6.3 and 6.4 show in detail the effect of allowing successively more particles to be exchanged between the clusters for L = 12. Figure 6.3 shows the phase shifts for the Volkov interaction 2 and NEX is the number of particles exchanged (n). The zero energy values of all these phases are the same (see table 6.1) but have been separated here by intervals of π for clarity. Figure 6.4 gives the phase shifts for the B_1 potential with the same notation. It is seen that the effects of exchange are monotonic with respect to increasing the value of n and each contribution is approximately

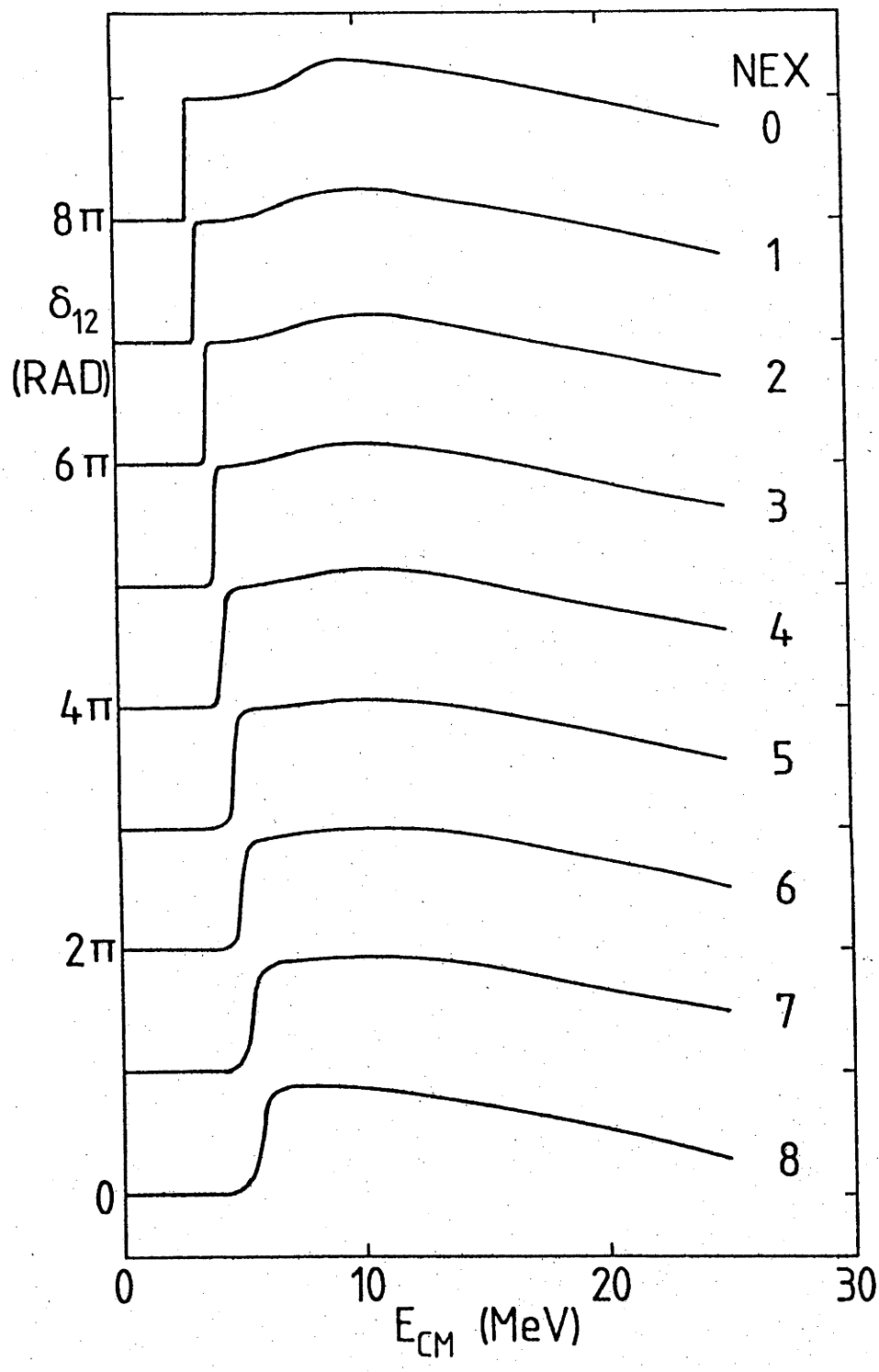

FIGURE 6.3 L = 12 phase shift for ^{16}O - ^{16}O scattering for different particle exchange approximations and a Volkov force 2. NEX is the number of particles exchanged and the phases have been separated by intervals of π for clarity.

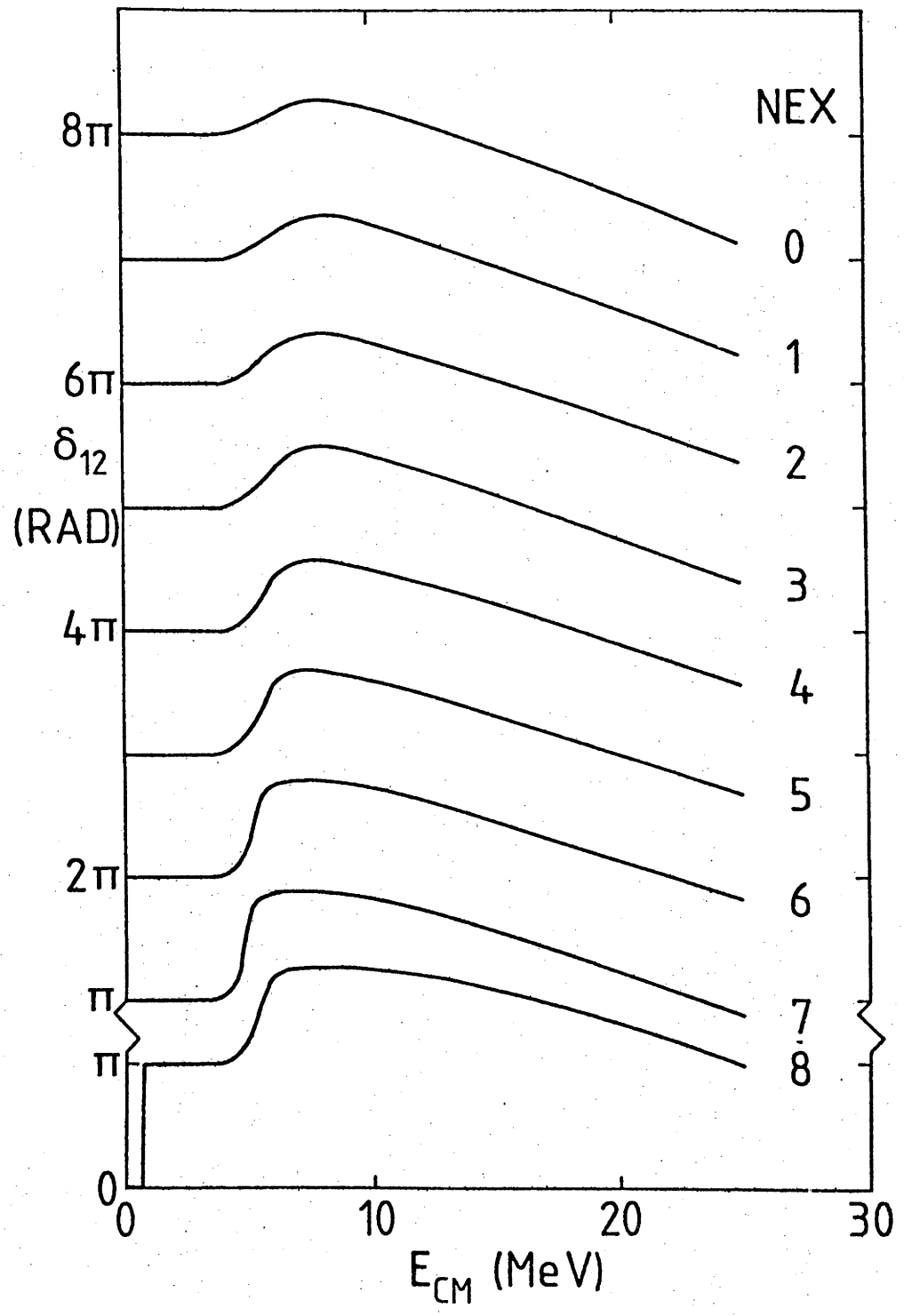

FIGURE 6.4 Same notation as fig. 6.3 but with a Brink and Boeker force B_1.

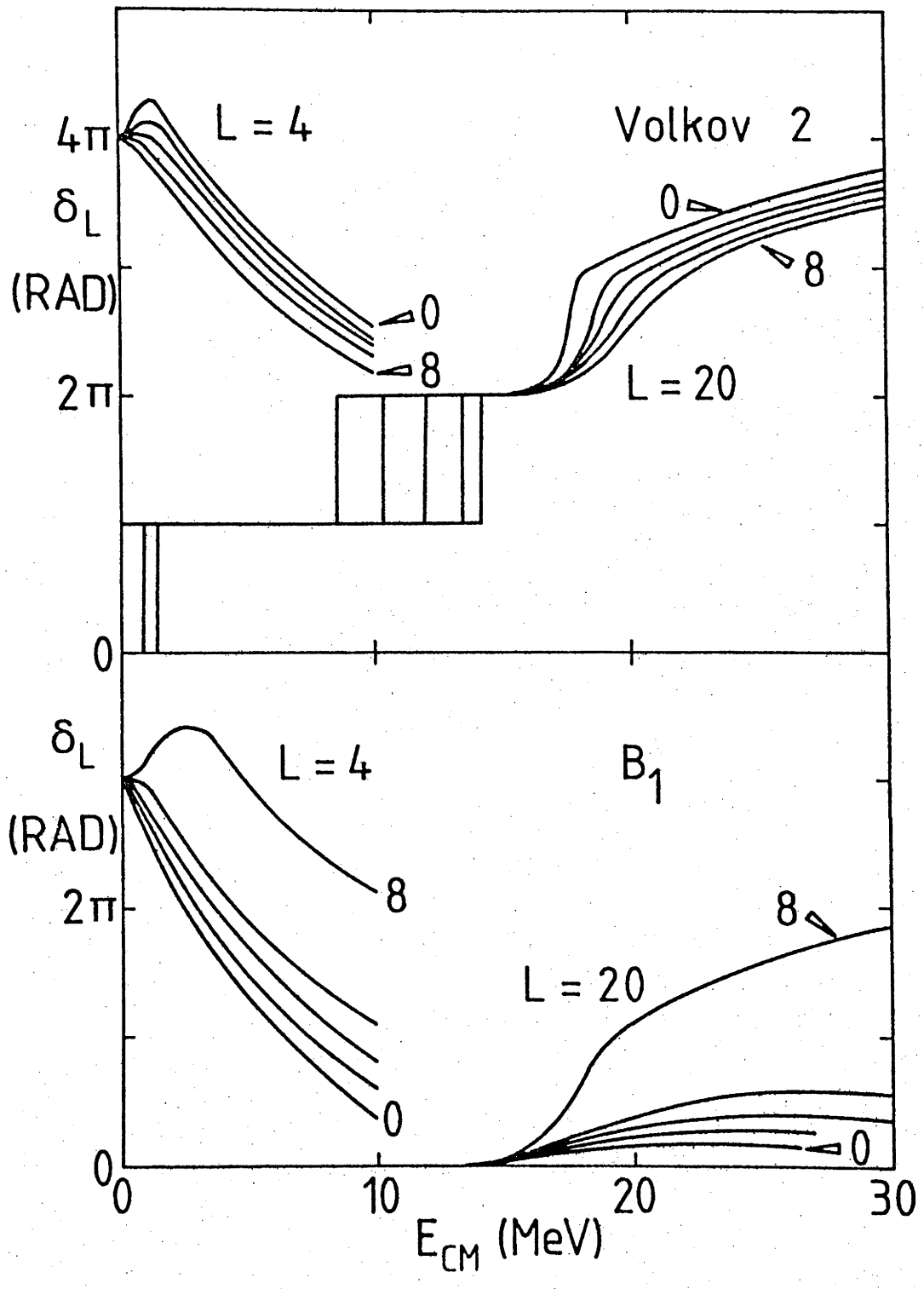

FIGURE 6.5 L = 4 and 20 phase shifts for ^{16}O - ^{16}O scattering for different n-particle exchange approximations. The numbers adjacent to the curves are the n-value for that result and the intermediate curves correspond to n = 2, 4, 6 in sequence with the n = 2 curve nearest the n = 0 curve. The forces are the same as in fig. 6.2.

equal although for the B_1 interaction increasing the value of n from 7 to 8 gives rise to the greatest change in the phase shift. This will be discussed further in chapter 7. These results are contrary to earlier calculations, emphasise the importance of making consistent approximations and show that contributions from all terms may be important.

Figure 6.5 shows the phases for L = 4 and 20 and n = 0, 2, 4, 6 and 8 for both forces. It should be noted that for the Volkov force and L = 20 the resonance energies corresponding to $\delta_L = \pi/2$ and $3\pi/2$ increase monotonically from n = 0 to n = 8. It is seen that the above features occur throughout the angular momentum range of interest.

The equivalent diagrams using the inconsistent approximations (4.3.8) can not in general be drawn for odd values of n since the overlap matrix has negative diagonal elements giving rise to unphysical complex eigenenergies. This problem was noticed by Ando *et al* (1975) and is discussed in chapter 7.

§6.4 Bound and Forbidden States

As mentioned earlier, the BD method used in the present work automatically finds any bound states which may exist. This is because near the bound state energies, the logarithmic derivative of the wave function changes rapidly through all possible values. This means that for *every* choice of the boundary condition parameter the BD method will find eigenvalues very close to the bound states so that such states are easily recognised.

For the simple case of potential scattering, these negative energy states (if they exist) have radial quantum numbers (i.e. number of nodes) 0, 1, ..., etc., counting from the lowest energy state, in addition to the angular momentum quantum numbers of the original basis states, namely L and M. For some values of L, some of these quantum numbers will be forbidden (see §4.2) although the radial form of the wave functions will not be

identical to the corresponding Pauli forbidden state. This is because the ion-ion interaction is not a h.o. well. However, it is possible that the bound state solutions are very similar to the redundant solutions so that on diagonalisation they are projected to high energies. This is because the eigenstates must be orthogonal to the forbidden states in the fully antisymmetric calculation. The removal of otherwise permitted bound states has been noted before (Weiguny 1977) and studied in detail in the case of a single redundant solution (Englefield and Shoukry 1974).

Table 6.2 shows this antisymmetrisation effect for the L = 12 bound states and lowest resonance using the Volkov force 2 (no bound states exist for the B_1 interaction). In the direct or n = 0 approximation, there are eight bound states, six of which have forbidden quantum numbers. As n increases, the higher bound states and the lowest resonance increase in energy whereas the lowest state decreases in energy until for n = 8 the six lowest states "disappear". In fact, after the diagonalisation, these states generally "appear" as very large positive or negative eigenenergies being the null-state solutions which may appear at any energy.

As the number of exchanged nucleons increases, the eigenenergies of the bound states with allowed quantum numbers and the lowest resonance (or quasi-bound state) all increase in energy in approximately equal steps. This is shown explicitly by the bottom row of table 6.2 which gives the energy shifts of the $E_{CM} \simeq 4$ MeV resonances as n increases from 0 to 8. This linear change in the resonance energy as the value of n increases supports the conclusion drawn in §6.3 that all particle-exchange terms need to be considered.

Only when n = 8 are the states with forbidden quantum numbers projected out of the energy range of interest. This is because it is only when the wave functions are fully antisymmetric that there are forbidden states. The part of the exchange operator that ensures orthogonality to the forbidden states must be equivalent to the orthogonality condition (OC)

TABLE 6.2 Bound state and lowest resonance energies for $^{16}0$ - $^{16}0$, L = 12 with a Volkov force 2 for different particle exchange approximations, n = 0, 1, ..., 8. The last row gives the energy shift of the lowest resonance as n increases. Bound states are numbered from the most bound and all energies are in MeV.

Bound States and Resonance	n = 0	1	2	3	4	5	6	7	8
E_1	-143.4	-143.0	-143.1	-143.4	-144.3	-147.3	-153.8	-165.0	-
E_2	-118.4	-117.8	-117.7	-117.7	-117.5	-116.7	-116.3	-114.9	-
E_3	- 94.9	- 94.1	- 93.7	- 93.6	- 93.1	- 91.9	- 89.6	- 84.9	-
E_4	- 73.2	- 72.1	- 71.5	- 71.1	- 70.5	- 69.3	- 67.0	- 63.0	-
E_5	- 53.3	- 52.1	- 51.2	- 50.5	- 49.7	- 48.4	- 46.3	- 44.1	-
E_6	- 35.4	- 34.2	- 33.2	- 32.3	- 31.2	- 29.8	- 27.9	- 26.4	-
E_7	- 19.7	- 18.7	- 17.7	- 16.8	- 15.8	- 14.6	- 13.0	- 11.7	-10.8
E_8	- 6.6	- 5.9	- 5.2	- 4.5	- 3.8	- 2.9	- 2.0	- 1.1	- 1.0
$E_{res.}$	2.9	3.3	3.7	4.1	4.4	4.8	5.1	5.4	5.7
$\Delta E_{res.}$	-	.4	.4	.4	.3	.4	.3	.3	.3

and is only "switched-on" when n = 8. If the OC is important for the scattering, then a large change in the resonance energy and phase shift would be expected as the value of n increases from 7 to 8. That this is not true indicates that for this interaction the only significant effect of the OC is to remove some of the bound states.

For the B_1 interaction, there are no bound states or resonances for the direct potential $V_D(r)$ although when n = 8 a resonance suddenly "appears". This must be due to the OC, since other exchange effects are roughly linear in n. This suggests the general rule that when there are no bound states with forbidden quantum numbers then the OC is crucial in the low energy scattering region.

Finally, it is possible for one of the eigenstates with forbidden quantum numbers to appear in the positive energy region as a narrow resonance when n = 0 but which is projected out when n = 8. In the present problem this occurs for L = 20 when the coulomb repulsion is included and shows that care must be taken, when using the folding approximation (§3.4) in a microscopic model, to ensure that any resonances do not correspond to Pauli forbidden states. All these results are discussed further in chapter 7.

CHAPTER 7

DISCUSSION OF RESULTS AND APPROXIMATIONS

§7.1 The BD method applied to composite particle scattering

To assess the accuracy of the BD method for this application an independent test was used which did not rely on the commonly made assumption that the *stability* of the method is a measure of its accuracy. The phase shifts for the scattering from a simple potential ($V_F(r)$) were obtained using the BD method and compared with results from an optical model calculation with the same potential. It was found that the two methods could be made to agree to *any desired accuracy* by increasing the number of basis states. As mentioned in chapter 6 this was used to determine the minimum number of basis states and the condition being demanded that the agreement should be better than .05 radians over the whole energy range (0 - 30 MeV). This may be taken as the absolute accuracy of the phases presented here. Tables 5.1 and 5.2 show how the method is stable with respect to the number of basis states and the matching radius for α - α scattering. The latter requirement is demanded of the method since physical observables must be *independent* of an arbitrary division of configuration space.

The BD method gives close agreement with the MRM of Baye and Heenen 1974b. The major distinction between the two approaches is in the choice of basis states. The method presented here uses a set of relative motion states modified by exchange while the MRM uses the original GCM wave function and defines a basis by discretising the generator coordinate.

Both calculations also agree well with the experimentally determined phase shifts although this is rather easily achieved by adjusting the force parameters particularly the Majorana exchange component. There have been many other microscopic calculations of α - α scattering using various forms of the GCM or RGM (Horiuchi 1970, Lumbroso 1974, Friedrich *et al* 1974, Beck *et al* 1975) and there is good agreement between the various methods apart from differences due to the choice of the two-body force. Clearly the GCM wave functions are a useful model for studying composite particle scattering although up till now using simple h.o. shell model configurations.

The method presented here has some advantages. Firstly, since the integration over the generator coordinates is performed and this defines the *basis* states, the matching at the channel radius involves the true relative motion wave function and does not require an unknown asymptotic GCM weight function. This overcomes one of the main problems of the GCM and allows the GCM kernels, which are much easier to calculate than the equivalent RGM kernels, to be used for the exchange contributions. The phases have been shown to be independent of the matching radius overcoming a problem of an early attempt to use R-matrix methods (Horiuchi 1970) for cluster scattering.

Secondly, the BD method relies only on a diagonalisation of the Hamiltonian matrix in a linearly independent basis. Furthermore, it does not attempt to find the GCM weight function, which may diverge as the mesh size is decreased (Lumbroso 1974). This may give rise to only semi-convergence or convergence to the wrong results.

The BD method has been tested by allowing up to 15 basis states (4 are sufficient for the α - α case) with no indication of numerical instability. Theoretically such behaviour should not occur, because the basis states are orthogonal in the internal region as the asymptotic energy of the basis states, $E_\lambda = \left(\frac{\hbar^2 k_\lambda^2}{3\mu}\right)$ tends to ∞. For example if L = 0 and a = 5.5 fm then $E_{16} > 1000$ MeV and any overlap with the states in the energy region of

interest is negligible.

Finally it was found for the α - α scattering problem that the BD method gave good results with as few as three basis states plus the energy correction. This is to be compared with other methods in which the number of basis states used ranges from six in the MRM method (Baye and Heenen 1974b) and up to thirty two (Lumbroso 1974). This means that the BD method is very efficient in the use of computer storage and also computing time, since all matrix elements can be evaluated analytically except for the coulomb interaction for which a six-point numerical integration was found to be necessary.

The ^{16}O - ^{16}O results of figure 6.1 show that the BD method is suitable for larger cluster scattering. The phase shifts calculated using the coulomb interaction in the direct term only agree well with those due to Friedrich (1974, 1975) using the same approximation. Clearly then the BD method is a viable, properly convergent method which may be used to describe cluster scattering. Since the purpose of this work was largely to develop the method and to study exchange effects, the calculation including the full coulomb interaction has not been performed to save computer time.

The minimum number of basis states required for convergence depends on the initial form of basis states and in the α - α case it was found to be sufficient to use plane wave states. The ^{16}O - ^{16}O phases were calculated using a similar basis but now this choice is not as satisfactory, although the solution must still converge. For example, 35 and 15 basis states were required to calculate the L = 4 phase shift for the Volkov and B_1 interactions, respectively. This convergence compares unfavourably with the corresponding calculations of Canto (1977) (18 basis states) and Baye and Heenen (1977a) (10 basis states), respectively.

This fairly slow convergence is due to treating the whole interaction between the nuclei as the "perturbation" for which the plane wave basis states are diagonalised, i.e. the basis states are the eigenstates with

$V_{ij} = 0$ and no exchange kinetic energy terms. This may be overcome by using as a basis, relative motion states which are eigensolutions of the direct local potential and are readily calculated by integration of the Schrödinger equation. The "perturbation" using the Volkov force would now be relatively small and the projection of the redundant solutions would be well approximated by discarding the corresponding bound states. Another possibility, also not yet tested, would be to use the energy correction method for distant states, thus reducing the size of the basis required for the ^{16}O - ^{16}O scattering.

§7.2 Effects of Antisymmetrisation

All studies (Hodgson 1978) of the antisymmetrisation in composite-particle scattering show that the inclusion of full exchange has a significant effect. For the Volkov forces, diagrams 5.3, 5.4, 6.2 and table 6.2 show that not only are the phase shifts changed but also that some possible bound states of the system are projected out of the energy region of interest. In the α - α case, the exchange contributions act in the same way as an *attractive* potential, reducing both the resonance energies and their widths. For $L \geq 4$, these changes are very small so that the exact result is fairly well approximated by the no-particle exchange contribution. In the ^{16}O - ^{16}O case, with the Volkov force 2, the exchange terms act in the same way as a *repulsive* potential, increasing both the resonance energies and their widths. On the other hand, with the B_1 force, the exchange terms act as an *attractive* potential, increasing the phase shifts at all energies and may even create new resonances. These results show that full anti-symmetrisation contributes either repulsively or attractively depending on the effective interaction or the nature of the colliding clusters. This has been reported before (Schultheis and Schultheis 1978) although most calculations of the effective potential have used an interaction which

gives a repulsive exchange contribution.

Another important effect of the Pauli principle is to force the eigenstates to be orthogonal to the forbidden states. Just how important this orthogonality condition is, depends on the choice of the nucleon-nucleon interaction. If the Volkov forces are used, the relative motion states with forbidden quantum numbers are virtually always bound and figure 5.7 and table 6.2 show that projecting out the redundant states has little effect on the positive energy region. This has also been noted before (Buck *et al* 1977). Moreover the phase shifts are always increased by the additional constraint of the OC (Englefield and Shoukry 1974). For the effective interactions considered here, the OC is only important when states with forbidden quantum numbers are not bound.

It can now be understood why a Volkov interaction, which gives such a very deep direct potential, may be phase equivalent to the B_1 interaction which gives rise to a largely repulsive direct potential. Figure 7.1 is a plot of the direct potential $V_D(r)$ for the Volkov force 2 plus the usual centrifugal force. The "energy pockets" which can support bound or quasi-bound states become progressively deeper and the number of forbidden states increases as L is decreased. Thus the "available" depth of the potential well for each "non-forbidden" state with a given L value remains roughly constant i.e. about 30 MeV as for L = 24. This value is a lot closer to empirically determined optical potentials (see figure 3.2). The effective interaction for the B_1 force is more attractive than the direct potential alone and so the two effective two-body forces are approximately phase equivalent even though the folded potentials are very different.

The Pauli principle constrains the wave function in the innermost region ($r < 5$fm) to have a certain minimum number of nodes regardless of the potential in that region (Ando *et al* 1979). Thus the scattering is determined primarily by the surface region, where the two potentials are similar. For the deeply attractive direct potential arising from the

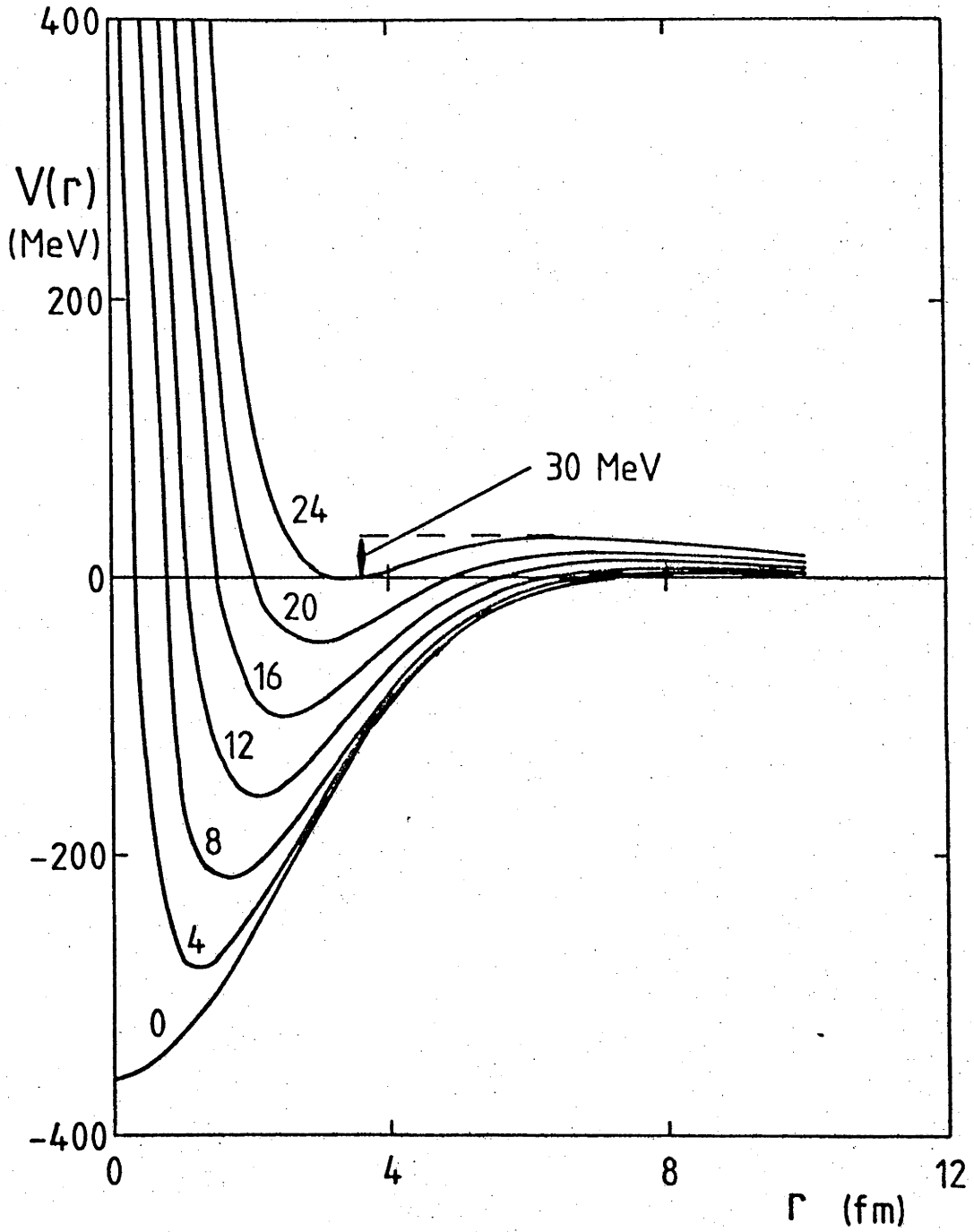

FIGURE 7.1 Direct potentials including the centrifugal term for ^{16}O - ^{16}O system and a Volkov force 2. The numbers refer to the L-value.

Volkov interaction, states with the correct number of nodes already exist in the low energy region and the OC simply removes the lower bound states. On the other hand the repulsive core of the B_1 direct potential shifts states with these quantum numbers to higher energies. The antisymmetrisation in this case has the important effect of allowing quasibound states to exist at lower energies giving rise to resonances in the region of interest. Therefore simply calculating the folded potential and comparing with an optical potential does not provide any criterion for choosing between effective interactions.

The forbidden states play another important role in the calculation via the modified Levinson's theorem (Swan 1955) which states that the zero-energy phase shifts must include the redundant states as if they were bound states. To illustrate this role the L = 0, 2 and 4 phase shifts for α - α scattering and the L = 4, 12, 20 and 24 phase shifts for ^{16}O - ^{16}O scattering have been calculated with the nuclear potential set to zero. Fig.7.2 shows that the kinetic energy terms are strongly repulsive for those L-values for which there are many redundant states. It should be noted that for convenience these phases have all been plotted with an E_{CM} = 0 value of zero. The modified Levinson's theorem shows that this is not the case and therefore the phases *as plotted* must have asymptotic values of: (i) in the α - α system; $\delta_0 \sim -2\pi$, $\delta_2 \sim -\pi$, $\delta_4 \sim 0$ and (ii) in the ^{16}O - ^{16}O system; $\delta_4 \sim -10\pi$, $\delta_{12} \sim -6\pi$, $\delta_{20} \sim -2\pi$ and $\delta_{24} \sim 0$. This repulsive nature of the kinetic energy terms may thus be regarded as a consequence of the Levinson's theorem.

In this work only the scattering of identical particles has been considered which means that only even angular momenta are involved. Therefore parity effects cannot be studied since in these cases the parity dependence is absolute. However, it is easy to see from eq. 4.4.2 how an odd-even angular momentum dependence can arise from the cancellation or

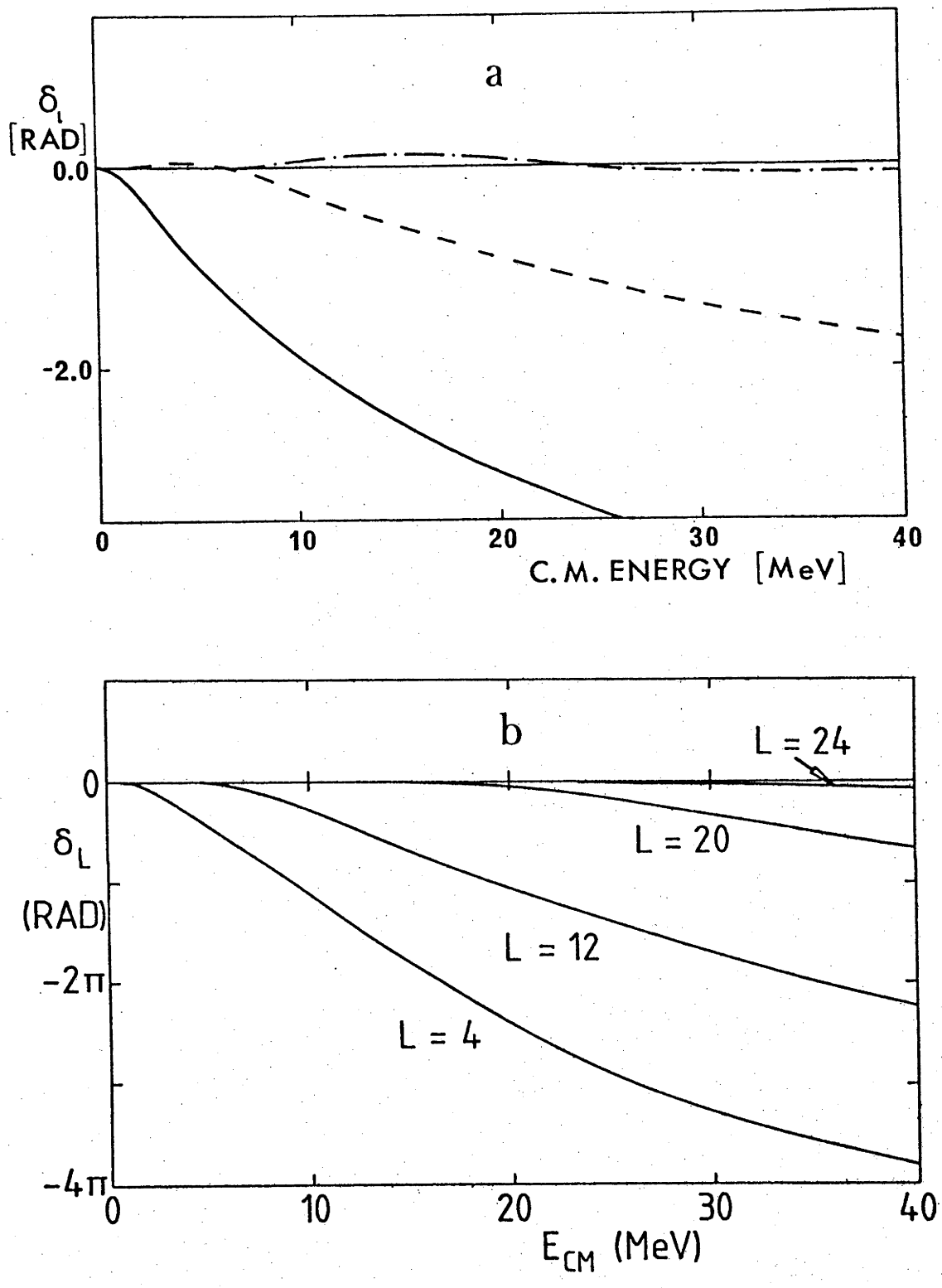

FIGURE 7.2 Phase shifts calculated with a zero effective interaction.
(a) α - α system. Solid curve is L = 0, dashed curve L = 2 and dot-dashed curve L = 4.
(b) ^{16}O - ^{16}O system. L values as marked, note the change of scale on the ordinate.

reinforcement of particle exchange terms. Baye *et al* (1977) have shown that the even-L effective potentials are generally deeper than odd-L potentials. This parity dependence can appear in the differential cross-section at large angles and parity-dependent optical potentials have been used successfully (Dehnhard *et al* 1978) to describe the large angle scattering of heavy-ions (Barrette *et al* 1978).

§7.3 Consistent particle exchange approximations

Many of the above manifestations of the Pauli principle have been noted before although comparisons between different effective potentials have only been made indirectly. The main new results arising from the present study are the calculation of the particle exchange approximations in a consistent way. In all other investigations of this problem, the exchange approximation has only been made in *one state vector* of the matrix elements which may lead to unphysical complex eigenenergies. This problem is related to the arbitrariness of the choice of the radial coordinate r. Failure to include exchange terms in both state vectors of the matrix elements leads to some possible choices of r, which would otherwise contribute to the direct term, becoming excluded. Only when the wave functions are *fully* antisymmetric are all choices of r equivalent and only one state vector of the matrix element needs to be antisymmetric.

Breaking down the full antisymmetrisation into a series of n-particle exchange contributions, it is found, for either choice of interaction and the positive energy region, that all the contributors are equally important (except when the OC plays a role). Therefore any approximate scheme must account for the dominant terms of each contribution. This is essentially what Ando *et al* (1975), LeMere *et al* (1977, 1979) and LeMere and Tang (1979) have done by using only the longest ranged terms from the RGM kernels. These are not just the 1-, 2-, ... etc. particle exchange contributions as these authors state but have contributions from *all* exchanges. This method,

however, has no *physical* justification and leads to serious problems in the $^{16}O - {}^{16}O$ example. This is almost certainly why Ando *et al* (1975) found that their method gave "exchange effects so large that we cannot reproduce the energies given by the RGM till we include the 5-exchange term". These difficulties stem from the fact that negative diagonal overlap matrix elements can be generated which is impossible for the norm of a vector in Hilbert space.

The correct interpretation of the particle exchange contributions shows that for composite particle scattering (i) any approximations must be included in both state vectors of the matrix elements and (ii) terms from all possible exchanges must be included.

§7.4 Approximations

In this section some further results are presented which were derived using approximations based upon the methods developed in this thesis. In §7.4a the use of the folded potential as an approximation for the direct potential while in §7.4b and §7.4c, two approximate treatments of the exchange contributions are discussed.

§7.4a Folded Potentials

In the cases considered in the present work, the direct potentials $V_D(r)$ were relatively easily determined analytically. This is because closed shell nuclei have been assumed so that their wave functions may be represented by a single Slater determinant. To treat more complicated nuclei using this model, it would be convenient to have a good approximation for the direct potential. For this purpose, the folded potential $V_F(r)$ has been considered, which is easy to evaluate, requiring only the single particle densities of the two nuclei.

The folded potentials for the α - α and ^{16}O - ^{16}O systems are plotted in figures 3.1 and 3.2. The phase shifts for L = 4, 12 and 20 for both the Volkov 2 and B_1 forces were calculated using only the folded potential and are plotted (solid curves) in figure 7.3. Also shown (dashed curves) are the corresponding phases calculated with the direct potential $V_D(r)$. The coulomb interaction has been included in both cases. The folded potential assumes the approximation that the centre-of-mass of each cluster is coincident with the centre of the single particle potentials. When the folded potential is used instead of the direct potential, there is a positive shift of about 1 MeV of the eigenenergies for *both* the Volkov and B_1 interactions.

In any nuclear model so far employed in this type of calculation, the experimentally determined ground and excited state energies are not found to this accuracy. Therefore the folded potential may be used as a good approximation to the direct potential until more accurate nuclear models are employed.

§7.4b Exchange Approximation Using Inelastic Channels

An approximation method derived from the Laplace expansion of the wave function $\phi(R, r_i)$ will now be discussed. In all of the exchange terms, there are single particle states, where the nucleon is on the "wrong" side, i.e. $\psi_j(r_i + R/2)$ instead of $\psi_j(r_i - R/2)$ and *vice versa*. This single particle state may be expanded in terms of the complete set of states on the "right" side:

$$\psi_j(r_i + R/2) = \sum_k^{\infty} a_{ik}(R)\ \psi_k(r_i - R/2). \qquad (7.4.1)$$

In this way each exchange term may be expressed as a series of core excited states of the original nucleus with the ground states as the first term. The single particle states $\psi_k(r_i - R/2)$ may have different angular

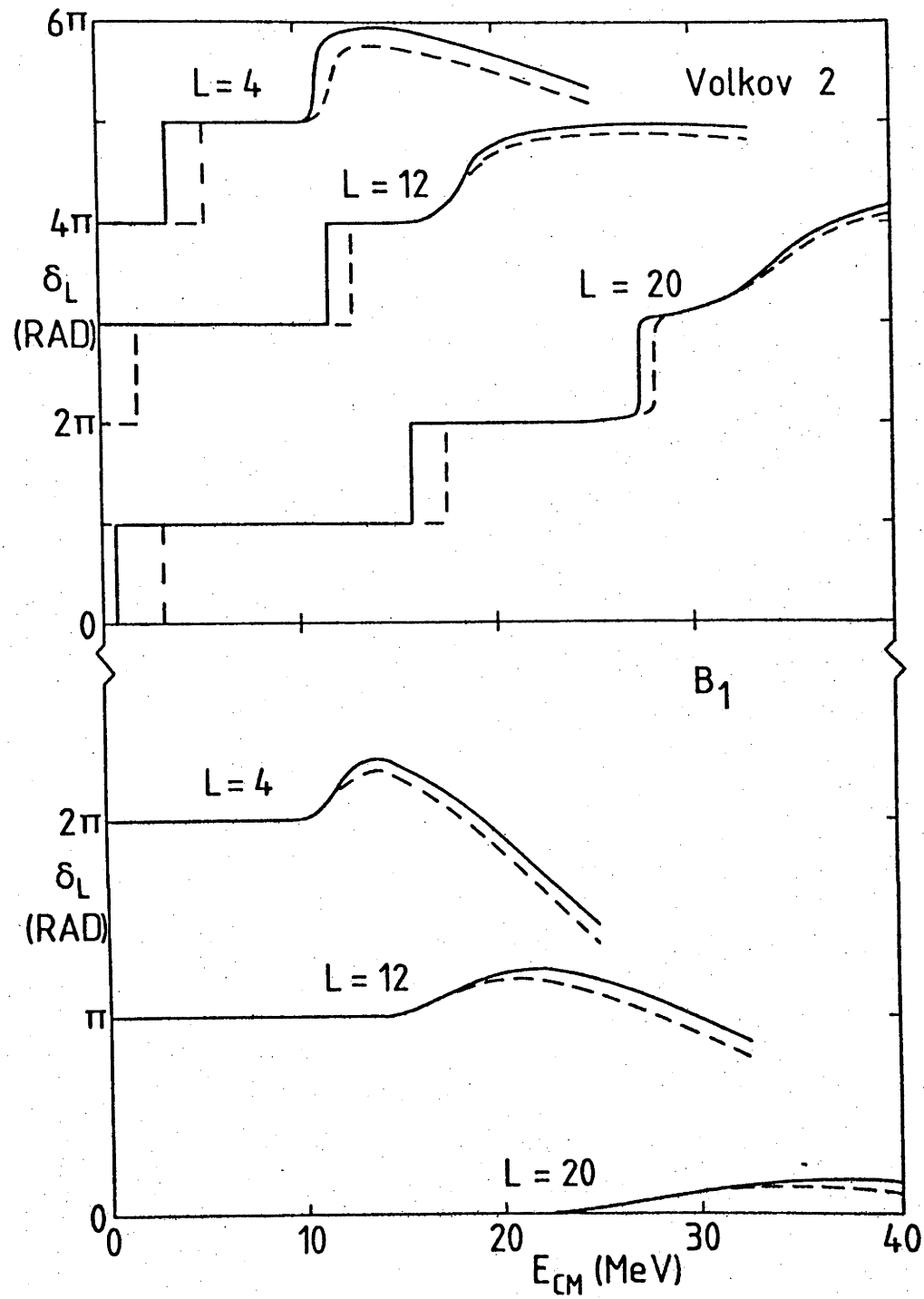

FIGURE 7.3 L = 4, 12, and 20 phase shifts for ^{16}O - ^{16}O scattering using the direct and folded potentials. Solid curves are results using $V_F(r)$ and dashed curve using $V_D(r)$. The upper phases are for a Volkov force 2 and the lower phases for the B_1 force. The coulomb interaction is included.

momentum quantum numbers so that the coefficients $a_{ik}(R)$ must be such that the total angular momentum remains constant. Therefore the exchange terms have been expressed as a series of inelastic channel wave functions, which form a complete set. Consequently, if a multichannel calculation is performed involving all possible inelastic channels, all terms are included and antisymmetrisation cannot change the results after diagonalisation.

The single channel elastic scattering calculation reproduces the experimentally determined phase shifts very well at low energies. At these energies all inelastic channels are closed and will therefore have little effect. If the expansion (7.4.1) converges quickly, the inelastic channels with the lowest thresholds should account for the antisymmetrisation effects in the energy range of interest. To test this hypothesis a coupled channels calculation has been performed for the α - α scattering. All excitations up to $2\hbar\omega$ that can be reached *directly* using the two-body Volkov force 6 were included. These are the $(1s)^3(2s)$ and $(1s)^3(1d)$ configurations. The $(1s)^3(1p)$ configuration is a simple c.m. excitation and does not give rise to an inelastic channel. The $(1s)^2(1p)^2$ configuration requires a two-step process.

The 0_2^+ excitation results in a two-channel problem and the 2_1^+ excitation results in a 4-channel problem. In the region of interest, $E_{CM} < 30$MeV, and for the Volkov force 6, all these channels are *closed*. In this case, the n.b.c. parameters of the closed channels are known and the BD method requires a single iteration on the open channel. Using the method described by Ahmad *et al* (1976a) the BD method is still straightforward and converges rapidly, requiring only small modification of the method described in §2.5.

Phase shifts for the L = 2 elastic scattering were calculated with and without the inclusion of these channels and are plotted in figure 7.4. The full lines are the results from a fully antisymmetric calculation with only the elastic channel. The dashed curves are the corresponding phases

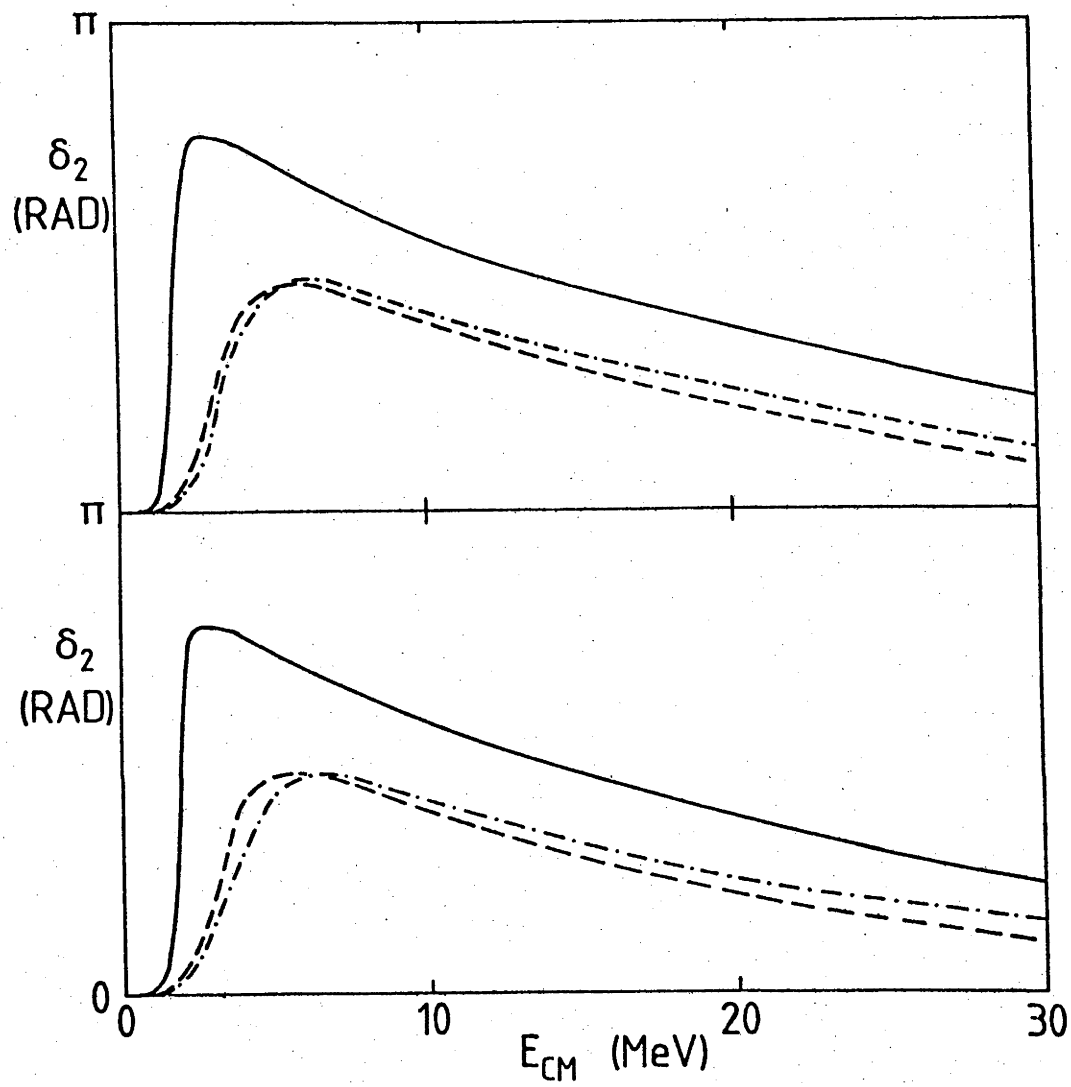

FIGURE 7.4 L = 2 phase shift for α - α scattering including closed inelastic channels. Solid curve is the exact result of the elastic scattering only calculation and the dashed curve the result using just the direct potential. The dot-dashed curve is the result of including an inelastic channel with no-exchange. The upper phases are for the 0_2^+ inelastic channel and the lower phases the 2^+ inelastic channel.

using only the direct potential and the dot-dashed curves are the phases with the inelastic channels included. Clearly these channels have a small effect.

This is not surprising, since the thresholds for these inelastic channels are in the region of 35 MeV. However, the small effect also indicates that the expansion (7.4.1) must converge slowly. Thus, this method is unlikely to represent a useful procedure for the approximation of the exchange terms.

§7.4c Exchange Approximation Using an Effective Q-Value

Another method tested as an approximation for the exchange terms involves the use of an effective Q-value similar to that employed by Seglie *et al* (1979). This is very easy to include in the BD method involving only the addition of an energy Q to the eigenenergies before matching the internal wave function to the external solution.

This is an entirely *ad hoc* procedure but the energy Q may be interpreted as that required to distort the nuclei so that the Pauli principle is satisfied.

The α - α scattering phase shifts for L = 0 and 2 were calculated using the direct potential and an effective Q value of -2 MeV and are the dot-dashed curves plotted in figure 7.5. The value of -2 MeV was chosen to reproduce the resonance energy for L = 2. The solid curves are the exact phases and the dashed lines are those for just the direct potential. In this case, the Q-value of -2 MeV indicates that the internal energy of the compound system is lower than that of the two α-particles so that the Pauli exchange contributes attractively. Clearly, not only can this procedure give a reasonable approximation but it is also easy to implement.

This *ad hoc* method can only be justified if such a Q value can be estimated from the model. However, the knowledge that such a simple device can give improved results may indicate the types of approximation that are required.

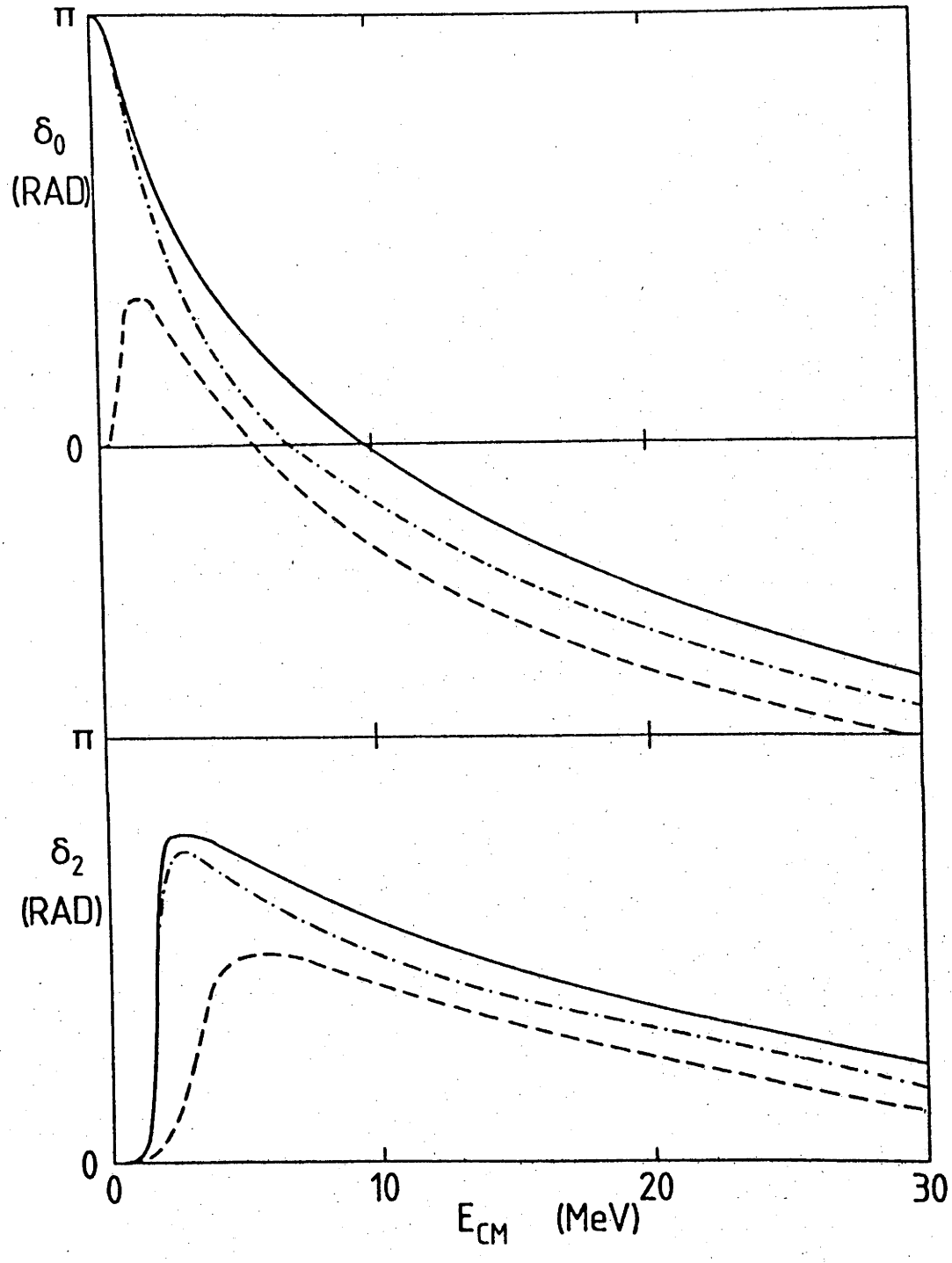

FIGURE 7.5 L = 0 and 2 phases for α - α elastic scattering using an effective Q-value. The solid curves are the exactly anti-symmetric results. The dashed curves are the results using just the direct potential and the dot-dashed the results using the direct potential plus an effective Q-value of -2MeV.

CHAPTER 8

SUMMARY AND CONCLUSIONS

This chapter is a brief summary of the methods developed in this thesis and of the main results and conclusions. A few possibilities for further investigations are suggested.

Previously, the *natural boundary condition* (NBC) methods have been shown to be both properly convergent and accurate, when applied to nuclear and atomic scattering. Furthermore, for any given basis, the extra constraint of natural boundary conditions guarantees that a minimum number of basis states are required.

The use of the generator coordinate method (GCM) to generate a set of *basis states* with a suitable asymptotic form, has allowed NBC methods to be applied to the problem of composite particle scattering. This method has been applied to α - α and ^{16}O - ^{16}O elastic scattering and compares well with both other calculations and experiment. This is an important step because in more realistic calculations of heavy-ion reactions, many channels will need to be taken into account explicitly, so that the number of basis states must be kept to a minimum. In the present work, only elastic and closed inelastic channels have been considered but earlier calculations using the NBC methods have demonstrated, for similar systems, that coupled open channel problems are readily solved.

Most of the problems associated with microscopic calculations arise from the effect of Pauli exchange interactions between the colliding nuclei. However, the use of the GCM kernels allows these terms to be calculated

fairly easily. To try and understand how the antisymmetrisation may be approximated, the exchange contributions have been studied in detail.

Firstly, by ignoring nucleon exchange between the clusters altogether, it has been shown that a direct potential may be defined. This direct potential is closely related to the well-known folded potential, which is derived by making the approximation that the centres-of-mass of the clusters coincide with the centres of the single particle wells, i.e. the c.m. motion of the clusters is ignored. It was found that this approximation results in a small error for ^{16}O - ^{16}O scattering. In lighter systems (e.g. α - α) this error is expected to be larger but in these cases it is easier to evaluate the direct potentials and there is no need for the folding approximation. The direct potentials arising from the two effective interactions considered in the thesis are very different, either supporting many bound states (Volkov force 2) or no bound states at all (B_1 interaction). However, on full antisymmetrisation, these effective interactions become nearly phase equivalent. This is because the Pauli principle largely determines the shape of the wave function in the innermost region, where the potentials differ by a large amount, so that the scattering is primarily determined by the potentials at the surface region where they are similar.

Secondly, analysis of the antisymmetrisation in terms of the number of nucleons exchanged between the clusters shows, contrary to earlier attempts which have been shown to be inconsistent, that the phase shifts change monotonically as more particles are exchanged. Furthermore, all exchange contributions are important because, with each extra exchanged particle, more of the indistinguishable elastic channels are opened. This somewhat paradoxical result is a feature of the microscopic model and arises from the arbitrariness of the definition of the relative separation. An analysis in terms of particle exchange also allows the importance of forbidden states to be estimated. It was found that if the states with forbidden quantum numbers are all bound then the orthogonality condition

(OC) has only a small effect on the phase shifts. In the α - α example this was calculated explicitly while in the ^{16}O - ^{16}O case it was inferred from the behaviour of the bound states and phase shifts. On the other hand, if there are no bound states associated with the direct potential, the OC is important and has a large effect on the phase shifts.

Finally some approximate methods, for treating the contributions from nucleon exchange between the clusters, have been tested. The first method uses the fact that, if all inelastic channels are included, then the basis is complete and antisymmetrisation cannot affect the results after diagonalisation. The phases calculated indicate that very many channels would have to be included and so this approach is not likely to be useful. The second method uses an effective Q-value, in the elastic channel, to approximate for the change in internal energy due to the Pauli principle. This method gives improved results but at present is entirely *ad hoc*.

The results and conclusions of this work are now summarised:

(i) NBC methods can be extended to treat composite particle scattering and yield accurate results;

(ii) the Pauli principle is important for microscopic calculations of cluster scattering;

(iii) the exchange terms may behave attractively *or* repulsively depending on the effective two-body interaction;

(iv) any approximations regarding particle exchange between the clusters must be included in both state vectors of the matrix elements in order to be consistent;

(v) all particle exchange contributions are important;

(vi) the OC is important only when the states with forbidden quantum numbers are unbound;

(vii) effective nucleon-nucleon interactions giving rise to totally different direct potentials can be phase equivalent under antisymmetrisation.

Certain problems arising from this work which warrant immediate attention are: (i) the calculation of ion-ion effective potentials from the *dynamical* solution and the study of their energy dependence in terms of particle exchange; (ii) theoretical investigation of the effective Q approximation; (iii) investigation of the use of a basis other than plane waves for the relative motion of the two clusters, so that convergence is improved; and (iv) further calculations using the BD energy correction method for the same reason.

It would be interesting to apply these methods to a study of the energy and parity dependence of the ion-ion interaction in a system with different nuclei, and to compare this dependence with that arising from the inclusion of inelastic channels (MacKintosh and Kobos 1979). The expansion of the exchange terms in §7.4b suggests that the effects from each of these sources should be similar. It would also be interesting to investigate the use of more realistic forces, e.g. the Skyrme interaction, which has already been used with GCM wave functions (Brink and Stancu 1975). Some of these investigations are already in progress.

It is believed that the NBC methods developed in this thesis are a useful technique for composite particle scattering. Also a clearer understanding of the role of the Pauli principle in cluster scattering calculations has been reached, by a correct interpretation of the exchange terms. It is hoped that this understanding will lead to useful approximations for these terms.

APPENDIX A

ASYMPTOTIC FORM OF THE BASIS STATES

The basis states are

$$\Psi_{LM} = \int dR\phi(R) j_L(k_\lambda R) Y_{LM}(\Omega_R). \tag{A1}$$

For identical particle scattering $\phi(R)$ is the (2n x 2n) Slater determinant

$$\phi(R) = \frac{1}{\sqrt{(2n)!}} \begin{vmatrix} \psi_1(r_1-R/2)\ldots\psi_n(r_1-R/2)\psi_1(r_1+R/2)\ldots\psi_n(r_1+R/2) \\ \vdots \\ \psi_1(r_{2n}-R/2)\ldots\psi_n(r_{2n}-R/2)\psi_1(r_{2n}+R/2)\ldots\psi_n(r_{2n}+R/2) \end{vmatrix} \tag{A2}$$

where the ψ_i are harmonic oscillator (h.o.) orbitals multiplied by a spin-isospin wave function. This may be expanded into a series of products of (n x n) determinants by the Laplace method

$$\phi(R) = \frac{1}{\sqrt{(2n)!}} \left\{ \begin{vmatrix} \psi_1(r_1-R/2)\ldots\psi_n(r_1-R/2) \\ \vdots \\ \psi_1(r_n-R/2)\ldots\psi_n(r_n-R/2) \end{vmatrix} \times \begin{vmatrix} \psi_1(r_{n+1}+R/2)\ldots\psi_n(r_{n+1}+R/2) \\ \vdots \\ \psi_1(r_{2n}+R/2)\ldots\psi_n(r_{2n}+R/2) \end{vmatrix} + \ldots \right.$$

$$\left. + \begin{vmatrix} \psi_1(r_1+R/2)\ldots\psi_n(r_1+R/2) \\ \vdots \\ \psi_1(r_n+R/2)\ldots\psi_n(r_n+R/2) \end{vmatrix} \times \begin{vmatrix} \psi_1(r_{n+1}-R/2)\ldots\psi_n(r_{n+1}-R/2) \\ \vdots \\ \psi_1(r_{2n}-R/2)\ldots\psi_n(r_{2n}-R/2) \end{vmatrix} \right\}, \tag{A3}$$

where only the "direct" and "total-exchange" terms have been written explicitly. All the other terms contain functions of both +R/2 and -R/2 explicitly and are exchange terms. Inserting cluster coordinates, eq. (2.2.3), the h.o. orbitals all have arguments of the form

$$(R_{CM}\pm\frac{r}{2}\pm\frac{R}{2}+\rho_i). \tag{A4}$$

If $r\to\infty$ then only those determinants of eq. (A3) which have the same relative sign of r to R in each of their terms, i.e. all $(r+R)$ or all $(r-R)$, can contribute to the integral in eq. (A1). This is due to the short ranged nature of the h.o. orbitals. The only two terms of $\phi(R)$ which satisfy this criterion are the direct and total exchange terms and the asymptotic form of $\phi(R)$ is

$$\tilde{\phi}(R)=\frac{(1+P_r)}{\sqrt{(2n)!}}\exp(-4n\nu R_{CM}^2)\exp\{-\frac{n\nu}{2}(r-R)^2\}\begin{vmatrix}\psi_1(\rho_1)\ldots\psi_n(\rho_1)\\ \vdots\\ \psi_1(\rho_n)\ldots\psi_n(\rho_n)\end{vmatrix}\times\begin{vmatrix}\psi_1(\rho_{n+1})\ldots\psi_n(\rho_{n+1})\\ \vdots\\ \psi_1(\rho_{2n})\ldots\psi_n(\rho_{2n})\end{vmatrix}, \tag{A5}$$

where P_r is the parity operator acting on coordinate r. It should be remembered that the ρ_i are dependent via eq. (2.2.4). This factorised form of $\tilde{\phi}(R)$ arises only because h.o. states in their lowest configuration are assumed.

Substituting $\tilde{\phi}(R)$ into eq. (A1) gives the required asymptotic form

$$\Psi_{\lambda LM}=\frac{(1+P_r)}{\sqrt{(2n)!}}\,n!\;2^{3/2}\exp(-4n\nu R_{CM}^2)\,j_L(k_\lambda r)Y_{LM}(\Omega r)\tilde{\phi}_1\tilde{\phi}_2, \tag{A6}$$

where relations (5.2.6a), (5.2.6b) and (5.2.7) have been used and $\tilde{\phi}_1$, $\tilde{\phi}_2$ are normalised wave functions depending only on internal coordinates.

APPENDIX B

ANALYTIC FORM OF THE DIRECT AND FOLDED POTENTIALS AND THE EFFECTIVE INTERATION PARAMETERS

Assuming an effective interaction of the form

$$v_{ij}^{N} = V_0 \exp(-\beta r_{ij}^2)(w + mP_M) \tag{B1}$$

the direct and folded potentials are:

(i) α-α system

$$\left.\begin{aligned} V_D(r) &= 16V_0\left(w - \tfrac{m}{4}\right)\bar{\alpha}^{3/2}\exp(-\bar{\alpha}\beta r^2), \\ V_F(r) &= 16V_0\left(w - \tfrac{m}{4}\right)\alpha^{3/2}\exp(-\alpha\beta r^2), \end{aligned}\right\} \tag{B2}$$

where $\bar{\alpha} = \frac{4\nu}{4\nu+3\beta}$, $\alpha = \frac{\nu}{\nu+\beta}$ and ν is the range parameter of the harmonic oscillator (h.o.) single particle states.

(ii) ^{16}O-^{16}O system

$$\left.\begin{aligned} V_D(r) &= 16V_0\left(w - \tfrac{m}{4}\right)\bar{\alpha}^{3/2}\exp(-\bar{\alpha}\beta r^2)(\bar{\gamma}_1 + \bar{\gamma}_2\nu r^2 + \bar{\gamma}_3\nu^2 r^4), \\ V_F(r) &= 16V_0\left(w - \tfrac{m}{4}\right)\alpha^{3/2}\exp(-\alpha\beta r^2)(\gamma_1 + \gamma_2\nu r^2 + \gamma_3\nu^2 r^4), \end{aligned}\right\} \tag{B3}$$

now $\bar{\alpha} = \frac{16\nu}{16\nu+15\beta}$, $\alpha = \frac{\nu}{\nu+\beta}$ and

$$\left.\begin{aligned} \bar{\gamma}_1 &= \tfrac{\bar{\alpha}^2}{16}\left(256 + 288\tfrac{\beta}{\nu} + 105\left(\tfrac{\beta}{\nu}\right)^2\right), & \gamma_1 &= \tfrac{\alpha^2}{16}\left(256 + 320\tfrac{\beta}{\nu} + 124\left(\tfrac{\beta}{\nu}\right)^2\right), \\ \bar{\gamma}_2 &= \tfrac{\bar{\alpha}^3}{2}\left(\tfrac{\beta}{\nu}\right)^2\left(16 + 5\tfrac{\beta}{\nu}\right), & \gamma_2 &= \tfrac{\alpha^3}{2}\left(\tfrac{\beta}{\nu}\right)^2\left(16 + 6\tfrac{\beta}{\nu}\right), \\ \bar{\gamma}_3 &= \bar{\alpha}^4\left(\tfrac{\beta}{\nu}\right)^4, & \gamma_3 &= \alpha^4\left(\tfrac{\beta}{\nu}\right)^4, \end{aligned}\right\} \tag{B4}$$

The effective interactions used are in fact the sum of two terms of the form of eq. (B1). In the α-α case a Volkov (Volkov 1965) force 1 was used with a h.o. parameter $\nu = .27033$ fm^{-2}. In the ^{16}O-^{16}O example two potentials were used: (i) the Volkov force 2 with h.o. parameter $\nu = .20029$ fm^{-2} and (ii) the B_1 interaction of Brink and Boeker (1967) with h.o. parameter $\nu = .15432$ fm^{-2}. Table B1 lists the parameters of these effective interactions where $w_i = 1 - m_i$.

TABLE B1

Interaction	V_1 (MeV)	l_2 (fm^{-2})	m_1	V_2 (MeV)	2_2 (fm^{-2})	m_2
Volkov 1	-83.34	.3906	.56	144.86	1.487	.56
Volkov 2	-60.65	.30864	.65	61.14	.9803	.65
B_1	-140.6	.5102	.4864	389.5	2.0408	-.529

APPENDIX C

PARTICLE EXCHANGE OPERATORS FOR ^{16}O - ^{16}O

The fully antisymmetric wave function may be expanded into a series of products of two Slater determinants with particles (1-16) in one determinant and (17-32) in the other. If the columns of the first determinant are labelled 1-16 and those of the the second determinant 17-32, then all terms in the series may be obtained from the first (or direct) term using one or more permutation operators, P_{ij}, which interchange the single particle states appearing in columns i and j, respectively. This is essentially the Laplace expansion of the original 32x32 determinant into products of two 16x16 determinants with $1 \leq i \leq 16$, $17 \leq j \leq 32$.

The n-particle exchange operator, A_n, is the sum of all the terms in the series which involve a product of n of the permutations P_{ij} acting on n different columns in each determinant:

$$\left.\begin{aligned} A_n &= \sum_{i_1<i_2\ldots<i_n=1}^{16} \sum_{j_1<j_2\ldots<j_n=17}^{32} P_{i_1 j_1} P_{i_2 j_2} \ldots P_{i_n j_n}, \\ A_0 &= 1. \end{aligned}\right\} \qquad \text{(C1)}$$

Using the method outlined in §4.5 all products $A_1 A_n = A_n A_1$ may be calculated:

$$\left.\begin{aligned} A_1 A_0 &= A_1, \\ A_1 A_n &= \sum_{i=n-1}^{n+1} a_{ni} A_i, \end{aligned}\right\} \qquad \text{(C2)}$$

where the a_{ni} are integers given below in table C1.

TABLE C1

Coefficients	n=1	2	3	4	5	6	7	8
a_{nn-1}	256	225	196	169	144	121	100	81
a_{nn}	30	56	78	96	110	120	126	128
a_{nn+1}	4	9	16	25	36	49	128	-

Terms with $n > 8$ are included via the symmetry operator $(1 + P_R)$ for which $(1 + P_R)A_n \equiv (1 + P_R)A_{16-n}$.

Using the expansions (C2) and the procedure outlined in chapter 4 the n-particle exchange approximations to the GCM kernels may be calculated in terms of the exchange operators A_n, viz

$$(A_0 + A_1 + \ldots + A_n)^2 = \sum_{i=0}^{8} b_{ni} A_i, \qquad (C3)$$

where the b_{ni} are integers given in table C2.

TABLE C2

n \ i	0	1	2	3	4	5	6	7	8
0	1	-	-	-	-	-	-	-	-
1	257	32	4	-	-	-	-	-	-
2	14657	3632	1084	252	36	-	-	-	-
3	328257	121232	54984	23212	8516	2400	400	-	-
4	3640657	1777432	1048704	609980	336740	169100	73100	24500	9800
5	22720081	13702072	9694068	6913004	4848260	3277196	2155196	1478036	1251656
6	86848145	61798120	49774108	40694752	34085248	29382220	26240620	24435124	23846536
7	217721745	176312520	167478552	163061568	160552512	158997420	158047020	157526676	157361544

APPENDIX D

α-α HAMILTONIAN MATRIX ELEMENTS

The Hamiltonian matrix elements may be expressed analogously to eq. (5.2.) for the overlap matrix:

$$H_{ij} = \int_0^a r^2 dr \frac{(1+(-1)^L)}{2} \exp\left(\frac{-k_i^2}{8\nu}\right) j_L(k_i r) \Bigg\{ \left(\frac{9\hbar^2\nu}{m} + \frac{\hbar^2 k_j^2}{4m}\right) \frac{1}{2} \exp\left(\frac{-k_j^2}{8\nu}\right) j_L(k_j r)$$

$$\frac{-32\sqrt{2}}{5^{3/2}} \exp\left(\frac{-k_j^2}{5\nu} - \frac{6\nu r^2}{5}\right) \Bigg[\left(\frac{81\hbar^2\nu}{10m} + \frac{37\hbar^2 k_j^2}{100m} - \frac{12\hbar^2\nu^2 r^2}{25m}\right) j\left(\frac{4k_j r}{5}\right)$$

$$\frac{-12\hbar^2\nu}{25m} k_j r j_L'\left(\frac{4k_j r}{5}\right) \Bigg]$$

$$+3\sqrt{2} \exp\left(\frac{-k_j^2}{4} - 2\nu r^2\right) \left(\frac{6\hbar^2\nu}{m} + \frac{\hbar^2 k_j^2}{2m}\right) j_0(k_j r) \delta_{L0}$$

$$+V_0 \alpha^{3/2} \sum_{m=1}^{11} a_m \exp(-b_m k_j^2) \exp(-c_m r^2) j_L(d_m k_j r) \Bigg\}, \qquad \text{(D1)}$$

where the first terms correspond to the kinetic energy operator and the sum is the contribution from the effective interation given by eq.(5.2.9). The real coefficients a_m, b_m, c_m, d_m and α depend on the parameters of the force and are listed in table D1 with

$$\alpha = \frac{4\nu}{4\nu + 3\beta} . \qquad \text{(D2)}$$

TABLE D1

m	a_m	b_m	c_m	d_m
1	$2(4w+2b-2h-m)$	$\frac{1}{8\nu}$	$\alpha\beta$	1
2	$2\left\{\frac{2\nu}{\alpha(\nu+\beta)}\right\}^{3/2}(6w+6b-6h-9m)$	$\frac{1}{4\alpha(\nu+\beta)}$	$2\nu+\alpha\beta-\frac{\alpha\beta^2}{4(\nu+\beta)}$	$\frac{\beta}{2(\nu+\beta)}$
3	$2\left\{\frac{8\nu}{\alpha(5\nu+4\beta)}\right\}^{3/2}(-9w-6b+6h+6m)$	$\frac{1}{\alpha(5\nu+4\beta)}$	$2\nu+\alpha\beta-\frac{\alpha(2\nu+\beta)^2}{5\nu+4\beta}$	$\frac{2(2\nu+\beta)}{5\nu+4\beta}$
4	$2\left\{\frac{8\nu}{\alpha(5\nu+6\beta)}\right\}^{3/2}(-w-2b+2h+4m)$	$\frac{1}{\alpha(5\nu+6\beta)}$	$2\nu+\alpha\beta-\frac{\alpha(2\nu+3\beta)^2}{5\nu+6\beta}$	$\frac{2(2\nu+3\beta)}{5\nu+6\beta}$
5	$2\left\{\frac{8\nu}{\alpha(5\nu+4\beta)}\right\}^{3/2}(-6w-6m)$	$\frac{1}{\alpha(5\nu+4\beta)}$	$2\nu+\alpha\beta-\frac{4\alpha(\nu+\beta)^2}{5\nu+4\beta}$	$\frac{4(\nu+\beta)}{5\nu+4\beta}$
6	$2^{5/2}(6w+6m)\,\delta_{L0}$	$\frac{1}{4\nu}$	$2\nu+\alpha\beta$	0
7	$2\left\{\frac{4\nu+3\beta}{4\nu+4\beta}\right\}^{3/2}(3w+3m)$	$\frac{1}{8\nu}$	0	1
8	$2\left\{\frac{4\nu+3\beta}{5\nu+6\beta}\right\}^{3/2}(-6w-6m)$	$\frac{\nu+\beta}{\nu(5\nu+6\beta)}$	$2\nu-\frac{4\nu(\nu+\beta)}{5\nu+6\beta}$	$\frac{4(\nu+\beta)}{5\nu+6\beta}$
9	$2\left\{\frac{4\nu+3\beta}{2(\nu+\beta)}\right\}^{3/2}(3w+3m)\,\delta_{L0}$	$\frac{1}{4\nu}$	2ν	0
10	$2\left\{\frac{2(4\nu+3\beta)}{5(\nu+\beta)}\right\}^{3/2}(-6w-6m)$	$\frac{1}{5\nu}$	$2\nu-\frac{4\nu}{5}$	$\frac{4}{5}$
11	$2\left\{\frac{2(4\nu+3\beta)}{4\nu+5\beta}\right\}^{3/2}(6w+6m)\,\delta_{L0}$	$\frac{\nu+\beta}{(4\nu+5\beta)}$	2ν	0

APPENDIX E

α-α GCM KERNELS

(i) Overlap kernel

$$O(R,R') = \exp\{-\nu(R^2+R'^2)\}x2(\cosh(2\nu R.R')-4\cosh(\nu R.R')+3). \quad (E1)$$

(ii) Kinetic energy kernel

$$T(R,R') = \frac{\hbar^2\nu}{2m}\exp\{-\nu(R^2+R'^2)\}x4\{(12-\nu R^2-\nu R'^2)(\cosh(2\nu R.R')-4\cosh(\nu R.R')+3)$$
$$+2\nu R.R'(\sinh(2\nu R.R')-2\sinh(\nu R.R'))\}$$
$$-\frac{3\hbar^2\nu}{2m}O(R,R'). \quad (E2)$$

(iii) Potential energy kernel

$$V(R,R') = V_0\alpha^{3/2}\exp\{-\nu(R^2+R'^2)\}\Big\{(X_d+X_e)4\{\cosh\{(1-\frac{\alpha\beta}{2\nu})\nu R.R'\}$$
$$+\cosh\{(1+\frac{\alpha\beta}{2\nu})\nu R.R'\}-2\cosh(\frac{\alpha\beta}{\nu}\nu R.R')\}+(X_d+X_e)\{\exp(-\frac{\alpha\beta R'^2}{4})$$
$$+\exp(-\frac{\alpha\beta R^2}{4})\}$$
$$x\{-8\{\cosh(\nu R.R')-1\}+X_d\exp\{-\frac{\alpha\beta}{4}(R^2+R'^2)\}4\{\cosh\{(2-\frac{\alpha\beta}{2\nu})\nu R.R'\}$$
$$-2\cosh\{(1-\frac{\alpha\beta}{2\nu})\nu R.R'\}+\cosh(\frac{\alpha\beta}{2\nu}\nu R.R')\}+X_e\exp\{-\frac{\alpha\beta}{4}(R^2+R'^2)\}$$
$$x4\{\cosh\{(1-\frac{\alpha\beta}{2\nu})\nu R.R'\}+\cosh\{(1+\frac{\alpha\beta}{2\nu})\nu R.R'\}-2\cosh(\frac{\alpha\beta}{2\nu}\nu R.R')\}, \quad (E3)$$

where $X_d = 8w + 4b - 4h - 2m$, $X_e = 8m + 4h - 4b - 2m$ and $\alpha = \frac{\nu}{\nu+\beta}$.

APPENDIX F

MATRICES B, B^{-1} AND VARIOUS MATRIX ELEMENTS FOR ^{16}O-^{16}O

$$B = \exp\{-\frac{\nu}{8}(R^2+R'^2)\} \times \begin{bmatrix} X & F_\lambda X & Y & F'_\lambda Y \\ -F_\kappa X & (\delta_{\kappa\lambda}-F_\kappa F_\lambda)X & -F'_\kappa Y & (\delta_{\kappa\lambda}-F'_\kappa F'_\lambda)Y \\ Y & -F'_\lambda Y & X & -F_\lambda X \\ F'_\kappa Y & (\delta_{\kappa\lambda}-F'_\kappa F'_\lambda)Y & F_\kappa X & (\delta_{\kappa\lambda}-F_\kappa F_\lambda)X \end{bmatrix}, \tag{F1}$$

where:

$$X = Y^{-1} = \exp(\frac{\nu}{4}R.R'),$$

$$F_\lambda = \frac{\sqrt{\nu}}{2}(R_\lambda - R'_\lambda),$$

$$F_\lambda = \frac{\sqrt{\nu}}{2}(R_\lambda + R'_\lambda),$$

the λ, κ subscripts denote x, y, z and B is an 8x8 matrix.

The inverse of B is fairly tedious to find but straightforward in principle. Writing

$$B = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}, \tag{F2}$$

where the A_{ij} are 4x4 matrices, it is seen by inspection that

$$A_{12} = P_{R'}A_{11}\ ,\ A_{21} = P_R A_{11}\ ,\ A_{22} = P_R P_{R'} A_{11}\ , \tag{F3}$$

where P_R and $P_{R'}$ are parity operators acting on coordinates R and R', respectively. Writing

$$B^{-1} = \begin{bmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{21} & \bar{A}_{22} \end{bmatrix} \tag{F4}$$

it is easy to show that

$$\bar{A}_{12} = P_R \bar{A}_{11} \ , \quad \bar{A}_{21} = P_{R'} \bar{A}_{11} \ , \quad \bar{A}_{22} = P_R P_{R'} \bar{A}_{11} \tag{F5}$$

and only $\bar{A}_{11}$ need be calculated. Using the simple rules for block matrices (Ayres 1974)

$$\bar{A}_{11} = (A_{11} - A_{12} A_{22}^{-1} A_{21})^{-1} \tag{F6}$$

$$= \exp\left\{\frac{\nu}{8}(R^2+R'^2)\right\}$$

$$\times \begin{bmatrix} \dfrac{(1-F^2)X}{A} + \dfrac{\{1\}Y}{A\,C} & -\dfrac{F_\lambda X}{A} - \dfrac{\sqrt{\nu}R_\lambda Y}{A\,C}(\nu R.R'\sqrt{\nu}R.FX^2+\sqrt{\nu}R.F'A) \\ \dfrac{F_K X}{A} - \dfrac{\sqrt{\nu}R_K Y}{A\,C}(-\nu R.R'\sqrt{\nu}R.FX^2+\sqrt{\nu}R.F'A) & \dfrac{\delta_{K\lambda} X}{A} - \dfrac{\sqrt{\nu}R'_K\sqrt{\nu}R_\lambda}{A\,C}(A-\nu R.R'X^2) \end{bmatrix},$$

where $A = X^2 - Y^2$, $C = A^2-(\nu R.R')^2$ and

$\{1\} = -\sqrt{\nu}R.F\sqrt{\nu}R'.F\nu R.R'X^2+(\sqrt{\nu}R'.F\sqrt{\nu}R.F-\sqrt{\nu}R.F'\nu R.R')A+(\nu R.R')^2Y^2+\nu R.R'A$

hence B^{-1} using relations (F5).

The calculation of the Hamiltonian kernel requires the following matrix elements

$$\left.\begin{aligned} T(i,j) &= \{\phi_i| \ -\frac{\hbar^2}{2m}\nabla_j^2 \ |\phi'_j\} \ , \\ V(i,j,k,L) &= \{\phi_i\phi_j|u(s_{kL})|\phi'_k\phi'_L\} \ , \end{aligned}\right\} \tag{F7}$$

for all i,j,k,L in the range 1-8.

The kinetic energy terms T(i,j) need only be calculated for i,j in the range 1-4 as the matrix elements for all other values of i,j may be determined using the operators P_R and $P_{R'}$. Regarding T(i,j) as a 4x4 matrix it is easy to show that

$$T = \frac{\hbar^2\nu}{2m}\exp\{-\frac{\nu}{8}(R-R')^2\}\begin{bmatrix} 3-F^2 & F_\lambda(5-F^2) \\ -F_\kappa(5-F^2) & \delta_{\kappa\lambda}(5-F^2) - F_\kappa F_\lambda(7-F^2) \end{bmatrix} . \qquad \text{(F8)}$$

The potential term is more complicated but all matrix elements may be found from three cases (i) $i,j,k,L \leq 4$, (ii) $i,j,k \leq 4$ $L > 4$, (iii) $i,k \leq 4$ $j,L > 4$. Then

$$\begin{aligned} V(i,j,k,L) = I_0\Big\{ &\left(\bar{Z}_k\bar{\zeta}_i + A_2\delta_{ik}(1-\delta_{i1})\right)\left(\bar{\zeta}'_j\bar{Z}'_L + A_2\delta_{jL}(1-\delta_{j1})\right) \\ &+A_1\left(\delta_{kL}(1-\delta_{L1})\bar{\zeta}_i\bar{\zeta}'_j+\delta_{ij}(1-\delta_{i1})\bar{Z}_k\bar{Z}'_L+\delta_{kj}(1-\delta_{j1})\bar{\zeta}_i\bar{Z}'_L+\delta_{iL}(1-\delta_{i1})\bar{\zeta}'_j\bar{Z}_k\right) \\ &+A_1^2\left(\delta_{kL}(1-\delta_{k1})\delta_{ij}(1-\delta_{i1}) + \delta_{kj}(1-\delta_{j1})\delta_{iL}(1-\delta_{i1})\right)\Big\} , \end{aligned} \qquad \text{(F9)}$$

where indices of the Kronecker deltas are to be interpreted as modulo 4 integers . $A_1 = \frac{1+\alpha}{2}$, $A_2 = \frac{1-\alpha}{2}$, and for the three cases:

$$\left.\begin{aligned} &\text{(i)} \quad I_0 = \alpha^{3/2}\exp\{-\tfrac{\nu}{4}(R-R')^2\} , \\ &\bar{Z} = 1, F \quad , \quad \bar{Z}' = 1, F \quad , \\ &\bar{\zeta} = 1, -F \quad , \quad \bar{\zeta}' = 1, -F \quad , \\ &\text{(ii)} \quad I_0 = \alpha^{3/2}\exp\{-\tfrac{\nu}{4}(R^2+R'^2) - \tfrac{\alpha\beta}{4}R'^2\} , \\ &\bar{Z} = 1, F+A_1(F-F') \ , \ \bar{Z}' = 1, F'-A_1(F-F') \ , \\ &\bar{\zeta} = 1,-F+A_1(F-F') \ , \ \bar{\zeta}' = 1,-F'-A_1(F-F') \ , \\ &\text{(iii)} \quad I_0 = \alpha^{3/2}\exp\{-\tfrac{\nu}{4}(R-R')^2 - \tfrac{\alpha\beta}{4}(R+R')^2\} \ , \\ &\bar{Z} = 1, \ F-2A_1F' \ , \ \bar{Z}' = 1, -F+2A_1F' \ , \\ &\bar{\zeta} = 1, -F-2A_1F' \ , \ \bar{\zeta}' = 1, \ F+2A_1F' \ . \end{aligned}\right\} \qquad \text{(F10)}$$

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